Supporting Information

Highly Double Selective Nitration of Nitrostilbenes over Zeolite

Junhui Xu, Jianping Wei, Zheng Hao, Qingguo Ma and Xinhua Peng *

School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China. E-mail: xhpeng@mail.njust.edu.cn Fax: (+) 86-025-84317639; Tel: (+) 86-025-84315520

1. Experimental.

1.1 General Remarks

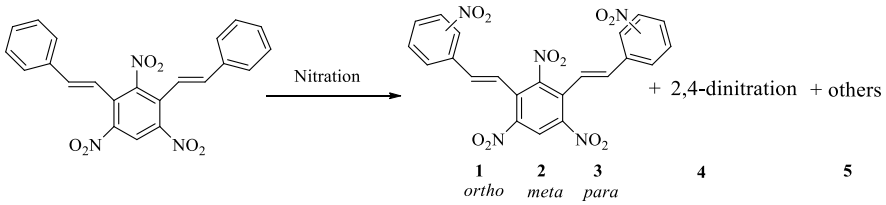
All nitrostilbenes were prepared in our laboratory.[1] All chemical reagents and solvents (analytical grade) were used as supplied unless otherwise stated. All experiments were monitored by thin-layer chromatography (TLC), TLC plates were visualized by exposure to ultraviolet light (254 nm). ^{1}H and ^{13}C spectra were recorded on a Bruker Avance III 500 MHz Digital NMR Spectrometer or 300MHz NMR Spectrometer, using $CDCl_3$ or DMSO-d_6 as a solvent and the chemical shifts were reported in δ (ppm) values. Coupling constants were reported in hertz (Hz). Mass spectra were obtained using an electrospray (ESI-TOF) mass spectrometer 6500 Series and a Bruker Daltonics flex Analysis instrument. Infrared spectra were recorded using Bruker Tensor 27 with the sample dispersed in a KBr pellet and were reported in terms of frequency of absorption (cm^{-1}). Elemental analysis was carried out on a Perkin-Elmer instrument. The melting points were determined on digital micro-melting point apparatus. Column chromatography was performed on silica gel (300-400 mesh) using ethyl acetate (EA)/ *n*-hexane (Hex).

1.2 General procedures for the nitration of nitrostilbenes

Representative synthetic procedure. Acetic anhydride (15.0 mL) was added to a stirring mixture of nitric acid (ca. 1.40 g, 68 %, 15.0 mmol), and H-Beta zeolite (0.20 g, SiO_2:Al_2O_3= 25) at 0 ℃ (the temperature rose temporarily to about 8 ℃ during this process). After a further 5 min, two drops of concentrated H_2SO_4 and then nitrostilbenes substrate (1.50 mmol) was added in small portions and the mixture was stirred for about 5-10 min at constant temperature. The zeolite was removed by suction filtration and washed with copious amounts of acetone when the reaction completed. Then, the mother liquor was poured into crashed ice (100.0 g) with stirring. The formed crude product was recrystallized from appropriate solvents or purified by silica gel chromatography.

2. Optimization details

Table S1. Optimization of nitration conditions [a]



Entry	Catalyst [b]	Nitrating agent	Temp. (℃)	Product distribution (yield mol%) [c]				
				1	**2**	**3**	**4**	**5**
1[d]	-	HNO_3/H_2SO_4	25	6	5	8	15	66
2	H_2SO_4	HNO_3/Ac_2O	0	32	6	20	12	30
3	H_2SO_4	HNO_3/Ac_2O	25	42	7	13	15	23
4	H_2SO_4	HNO_3/Ac_2O	45	33	5	12	12	38
5	H-Beta-25, H_2SO_4	HNO_3/Ac_2O	0	91	trace	3	trace	5
6	**H-Beta-25, H_2SO_4**	**HNO_3/Ac_2O**	**25**	**95**	**trace**	**trace**	**trace**	**4**
7	H-Beta-25, H_2SO_4	HNO_3/Ac_2O	45	88	trace	trace	4	7
8	H-Beta-45, H_2SO_4	HNO_3/Ac_2O	25	88	trace	trace	trace	11
9	H-Beta-300, H_2SO_4	HNO_3/Ac_2O	25	85	trace	trace	3	11
10	H-ZSM-5, H_2SO_4	HNO_3/Ac_2O	25	72	3	6	12	7
11[e]	K10	HNO_3/Ac_2O	25	35	4	20	11	30
12 [f]	H-Beta-25	NO_2/O_2	0	15	12	2	4	67
13 [f]	H-Beta-25	NO_2/O_3	0	16	11	2	6	65
14 [g]	H-Beta-25, H_2SO_4	HNO_3/Ac_2O	25	81	trace	4	7	7
15 [h]	H-Beta-25, H_2SO_4	HNO_3/Ac_2O	25	91	trace	trace	3	5

[a] All reactions were run using acetic anhydride (15.0 mL), catalyst: zeolite (0.20 g), H_2SO_4 (two drops, 98%), nitric acid (ca.1.40 g, 68%, 15 mmol), *trans*, *trans*-1, 3-distyryl-2, 4, 6-trinitrobenzene (1.5 mmol). [b] Commercial zeolites with different ratio of Si/Al, which were calcined at 500 ℃ for 8 h in air prior to use. [c] HPLC analysis (250 x 4.6 mm column (ZORBAX Eclipse XDB-C_{18}, 5 um)); solvent system-MeOH (50%): H_2O (50%), EDTA (0.1 mM)-citric acid (20 mM); flow rate-1mL/min; λ=254 nm; sample solvent-acetone (20 uL). [d] Traditional nitration method with sulfuric acids (10.0 mL) and nitric acid (1.0 mL, 95%).[e] A commercial product from Aldrich, calcined in air at 300 ℃ for 8 h prior to use, 0.20g. [f] Reactions with the NO_2/O_3 system were conducted at 0 ℃ using substrate (1.0 mmol), liquid NO_2 (1.5 mL), catalyst (0.20 g), and dichloromethane (20.0 mL) according to the Kyodai method, while those with the NO_2/O_2 system were carried out under an oxygen atmosphere. [g] Amount of catalyst was decreased to 0.08 g. [h] Amount of nitric acid was increased to 20 mmol.

3. Theoretical study

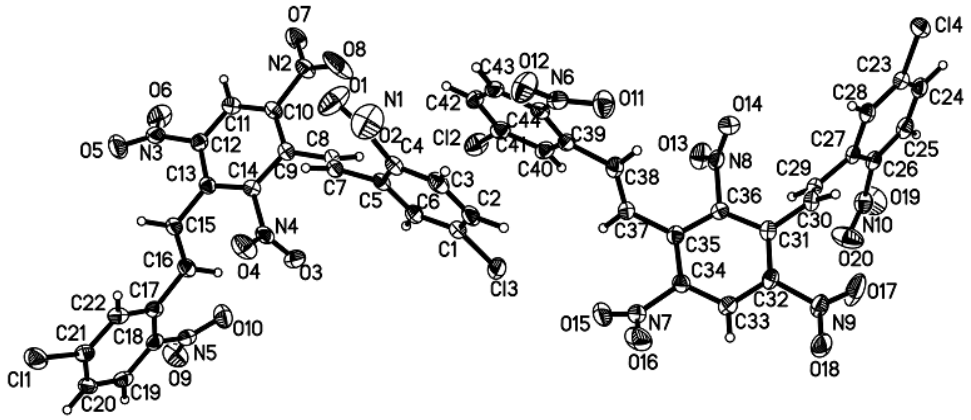
Calculations were performed with the Gaussian 03 (Revision D.01) suite of programs.[2] The geometric optimization of the structures were carried out by using the B_3LYP functional with 6-311+ G (d, p) basis set. All of the optimized structures were characterized to be true local energy minima on the potential energy surface without imaginary frequencies. The electrostatic potential (ESP) of related compounds were computed at the B3LYP/6-311+G (d, p) level of theory and processed with *multiwfn* [3].

4. Crystallographic data

Table S2. Crystallographic data and structure-refinement parameters for compound **2c** and **2e**.

Empirical formula	$C_{22}H_{11}Cl_2N_5O_{10}$ (**2c**)	$C_{24}H_{17}N_5O_{10}$ (**2e**)
CCDC number	9965295	999375
M_w [g mol^{-1}]	576.26	535.43
crystal system	Triclinic	Monoclinic
space group	P-1	C 2/c
a [Å]	7.9603(5)	24.48(2)
b [Å]	25.1844(15)	8.379(6)
c [Å]	12.0025(7)	11.878(9)
α [ ]	90	90
β [ ]	104.539(1)	106.275(14)
γ [ ]	90	90
V [Å^3]	2329.2(2)	2339(3)
Temperature/K	296	296
Z	4	4
Radiation type	MoKα	MoKα
ρ_{calcd} [mg m^{-3}]	1.643	1.521
M [mm^{-1}]	0.350	0.121
F (000)	1168.0	1104.0
crystal size [mm^3]	0.25 x 0.20 x 0.15	0.16 x 0.12 x 0.08
θ range [ ]	2.39 to 25.00	2.58 to 25.00
index ranges	$-9 \le h < 9$	$-28 \le h < 28$
	$-30 \le k < 30$	$-7 \le k < 9$
	$-14 \le l < 14$	$-14 \le l < 13$
reflections collected	18529	5631
independent reflections	8636 [R_{int} = 0.0162]	2042 [R_{int} =0.0520]
R [I > 2 σ (I)]	0.0374	0.0606
wR [I > 2σ (I)]	0.1023	0.1466
goodness-of-fit on F^2	0.591	1.040
largest diff. peak and hole [e Å^3]	0.448 and -0.347	0.316 and -0.245

a)



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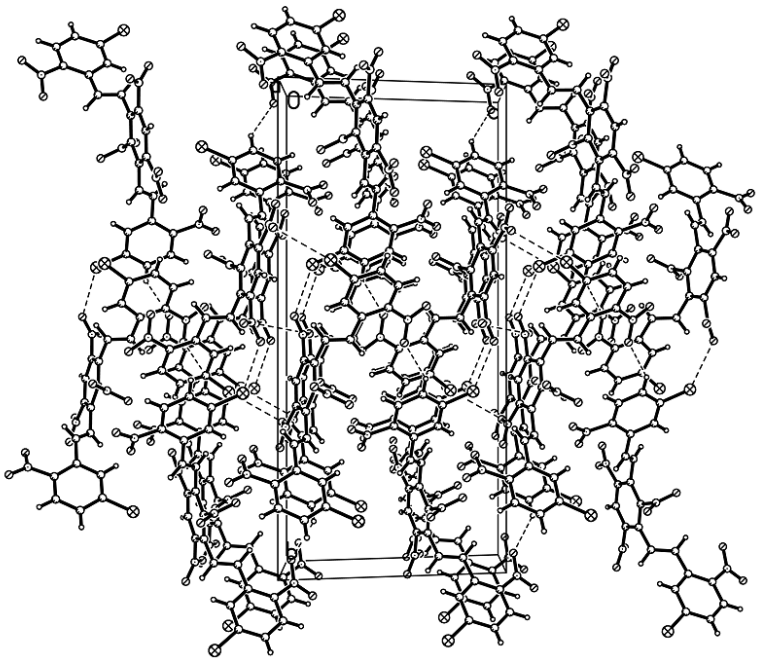
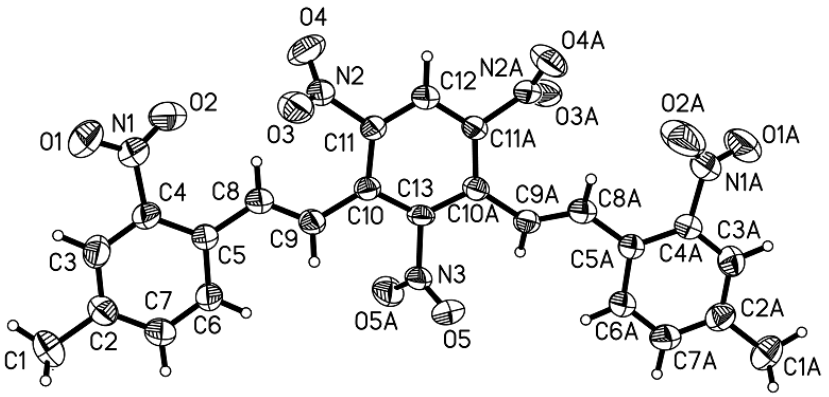


Figure S1. a) Thermal ellipsoid plot (50 %) and labeling scheme for **2c** (double moleculars). Hydrogen atoms are shown, but are unlabeled for clarity. b) Ball- and stack-packing diagram of **2c** viewed down the *c* axis. Dashed lines indicate strong hydrogen bonding.

a)



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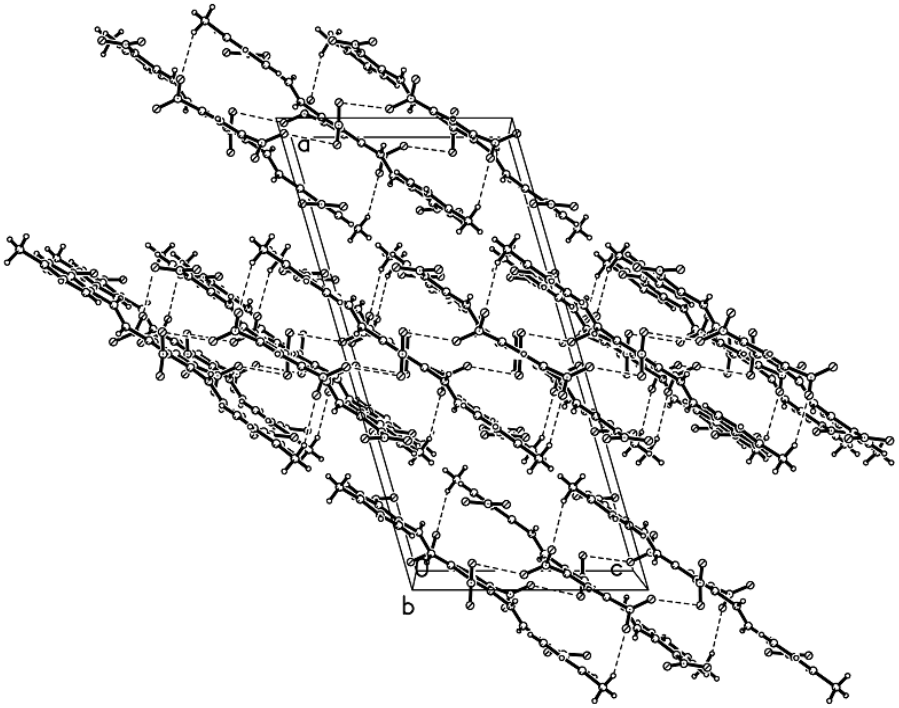


Figure S2. a) Thermal ellipsoid plot (50 %) and labeling scheme for **2e**. Hydrogen atoms are shown, but are unlabeled for clarity. b) Ball- and stack-packing diagram of **2e** viewed down the *c* axis. Dashed lines indicate strong hydrogen bonding.

5. Electrostatic potential analysis (ESP)

Table S3. Number of surface minima in *trans, trans*-1, 3-distyryl-2, 4, 6-trinitrobenzene: 20 (* represented the minimum point)

#	a.u.	eV	kcal/mol	X/Y/Z	coordinate(Angstrom)	
1	-0.01158868	-0.315344	-7.271434	-7.078202	0.207114	0.910898
2	-0.00969762	-0.263886	-6.084866	-6.384764	-2.516748	-2.039472
3	-0.01146811	-0.312063	-7.195778	-6.384764	-1.028977	1.961891
4	-0.00984634	-0.267933	-6.178186	-5.425235	-3.202017	-1.249563
5	-0.04107267	-1.117644	-25.771456	-4.349726	3.390203	2.147653
6	-0.04063416	-1.105712	-25.496312	-3.879238	4.729143	0.564227
7	-0.02973242	-0.80906	-18.655903	-3.156978	1.193923	2.941419
8	-0.00212539	-0.057835	-1.333596	-2.705634	-1.388801	-1.588075
9	-0.0331243	-0.901358	-20.784176	-0.00648	-4.092373	-1.101505
10	-0.03312017	-0.901246	-20.78158	0.006861	-4.096123	0.991126
11	-0.02310178	-0.628631	-14.495445	-0.066073	-1.915902	-2.799844
12	-0.02309398	-0.628419	-14.490548	0.089737	-1.904657	2.795943
13	-0.00215687	-0.058692	-1.353352	2.748837	-1.369213	1.608919
14	-0.02972722	-0.808919	-18.652641	3.140426	1.20186	-2.951165
15	-0.04061729	-1.105253	-25.485725	3.87564	4.690249	-0.643843
*16	-0.04110365	-1.118487	-25.790897	4.282356	3.503847	-2.096303
17	-0.00984867	-0.267996	-6.179645	5.521724	-3.224513	1.267436
18	-0.0097051	-0.264089	-6.089563	6.374962	-2.543827	2.015359
19	-0.01146706	-0.312035	-7.195124	6.422868	-1.038436	-1.953471
20	-0.01157917	-0.315085	-7.265465	7.114843	0.215954	-0.896213

Table S4. Number of surface maxima in *trans, trans*-1, 3-distyryl-2, 4, 6- trinitrobenzene: 23: (* represented the maximum point)

#	a.u.	eV	kcal/mol	X/Y/Z	coordinate	(Angstrom)
1	0.03239606	0.881541	20.327229	-9.460094	-3.366236	-0.123383
2	0.03175363	0.86406	19.924135	-9.113373	-0.153691	-2.168487
3	-0.00794342	-0.216152	-4.98418	-6.627144	-0.539174	1.261045
4	0.03140412	0.854549	19.704827	-6.54818	-4.746378	1.75077
5	-0.00595717	-0.162103	-3.737884	-5.483103	-2.313284	-1.572947
6	0.03702234	1.007429	23.230036	-4.48087	1.589857	-1.769402
7	0.03695618	1.005629	23.188523	-2.811865	-2.561276	1.618035
8	0.0373544	1.016465	23.438391	-2.564296	1.659787	-1.456932
9	0.01508255	0.410417	9.463699	-1.257742	-0.314038	2.078317
*10	0.04269692	1.161842	26.79061	-0.959066	3.655012	1.486286
11	0.02857445	0.77755	17.929323	-0.439985	1.137707	-1.702779
12	0.03795083	1.032694	23.812625	-0.011434	4.876329	0.050032
13	0.02856299	0.777238	17.922133	0.341581	1.13221	1.715481
14	0.04268656	1.16156	26.784106	0.992291	3.654792	-1.497029
15	0.01508018	0.410353	9.462213	1.167952	-0.304489	-2.069347
16	0.03737295	1.01697	23.45003	2.626486	1.664854	1.476807
17	0.03692555	1.004795	23.169305	2.801014	-2.540993	-1.631412
18	0.03703972	1.007902	23.240942	4.510702	1.576209	1.773366
19	-0.0059837	-0.162825	-3.754535	5.529519	-2.278707	1.610883
20	0.03144095	0.855552	19.727937	6.549556	-4.69003	-1.847774
21	-0.00801173	-0.21801	-5.02704	6.595019	-0.568299	-1.295886
22	0.0317636	0.864332	19.930391	9.11842	-0.159346	2.164609
23	0.03240257	0.881719	20.331318	9.484451	-3.323047	0.183148

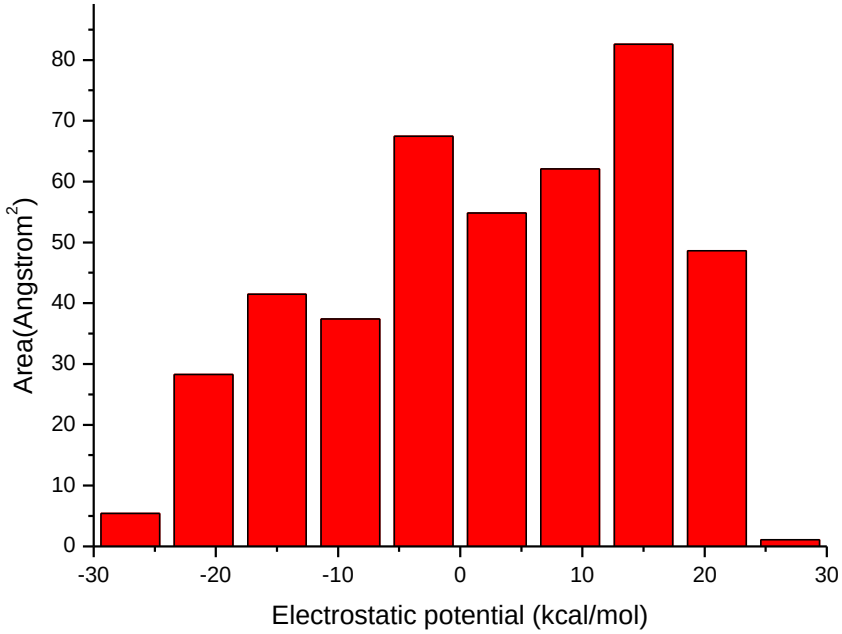


Figure S3. The electrostatic potential of compound *trans*, *trans*-1, 3-distyryl-2, 4, 6-trinitrobenzene quantitative distribution [B3LYP/6-311+ G (d, p), 0.001 electron/b^3 isosurface].

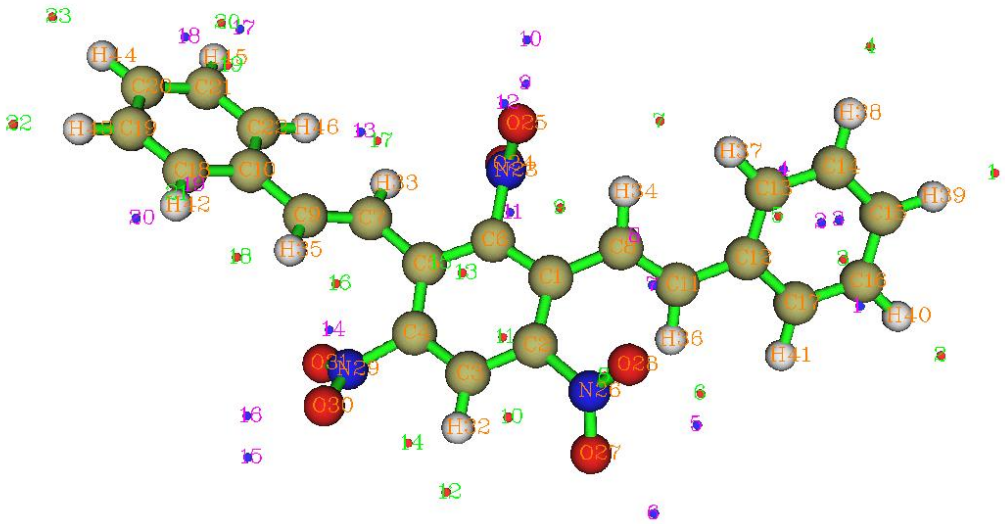


Figure S4. The distributed electrostatic potential surface maxima and surface minima of compound *trans*, *trans*-1, 3-distyryl-2, 4, 6-trinitrobenzene [B3LYP/6-311 G (d, p), 0.001 electron/b^3 isosurface], color coding: red points (electrostatic potential maximum points), blue points (electrostatic potential minimum points).

Table S5. Number of surface minima in *trans*-1-styryl-2, 4-dinitrobenzene: 12 (* represented the minimum point)

#	a.u.	eV	kcal/mol	X/Y/Z coordinate (Angstrom)		
1	-0.0072626	-0.197626	-4.557011	-5.188499	-0.994438	-2.199447
2	-0.0093204	-0.253621	-5.848183	-4.816734	0.0812	1.89652
3	-0.010132	-0.275705	-6.357408	-4.800656	1.536486	0.976434
4	-0.00234468	-0.063802	-1.471191	-1.441839	-1.323399	-1.772423
5	-0.0419577	-1.141728	-26.32679	-0.819365	3.592591	1.843573
6	-0.0304595	-0.828844	-19.1121	-0.687071	1.15392	2.917118
7	-0.0419034	-1.140248	-26.29268	0.106695	4.416187	0.178644
8	-0.0287326	-0.781852	-18.02852	1.560006	3.407375	-1.771363
9	0.01311225	0.356803	8.227414	1.682751	-1.761369	-1.937095
10	0.01250374	0.340244	7.8456	2.110411	-1.740078	2.077459
*11	-0.049551	-1.348351	-31.09127	7.177632	0.669321	-0.556379
12	-0.0488733	-1.32991	-30.66603	7.264146	-1.085272	-0.586379

Table S6. Number of surface maxima in *trans*-1-styryl-2, 4-dinitrobenzene: 16: (* represented the maximum point)

#	a.u.	eV	kcal/mol	X/Y/Z coordinate(Angstrom)		
1	0.03415878	0.929508	21.433271	-8.438888	-0.776948	-0.304033
2	0.03080976	0.838376	19.331895	-7.247279	-1.966637	0.59555
3	0.03291744	0.895729	20.654379	-6.788941	2.212274	-2.100967
4	0.03508236	0.95464	22.01278	-6.230706	-3.324864	1.534427
5	-0.006286	-0.171049	-3.944181	-4.771932	0.647297	1.265551
6	0.02925199	0.795987	18.354451	-4.796642	2.360123	-1.938037
7	-0.0032089	-0.087319	-2.013461	-4.414685	-1.247312	-1.683983
8	0.03536051	0.962209	22.187308	-1.991994	1.941966	-1.626005
*9	0.05214351	1.418897	32.717965	-0.24965	-3.435843	0.485211
10	0.03439852	0.936031	21.583698	-0.157893	1.021626	-1.449127
11	0.02305572	0.627378	14.46654	1.822362	-0.435322	-1.660422
12	0.04661116	1.268354	29.24664	1.958816	-3.784292	0.045182
13	0.02178442	0.592784	13.668853	2.244037	-0.547752	1.814715
14	0.03859082	1.05011	24.214195	2.261132	2.376679	1.276151
15	0.03122703	0.849731	19.593711	4.228757	-0.41585	-2.021896
16	0.03161797	0.860369	19.839013	4.624359	-0.416539	1.549262

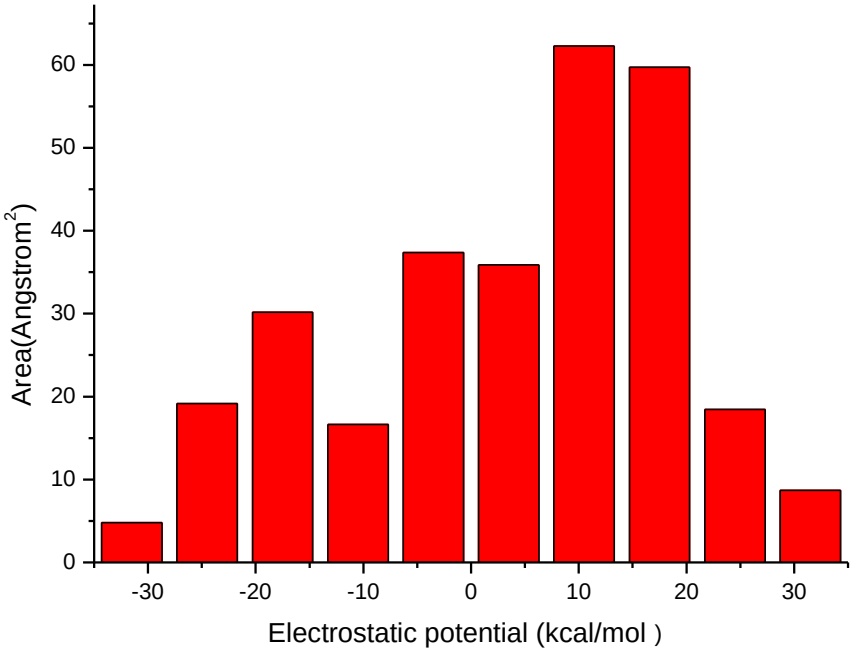


Figure S5. The electrostatic potential of compound *trans*-1-styryl-2, 4-dinitrobenzene quantitative distribution [B3LYP/6-311+ G (d, p), 0.001 electron/b^3 isosurface].

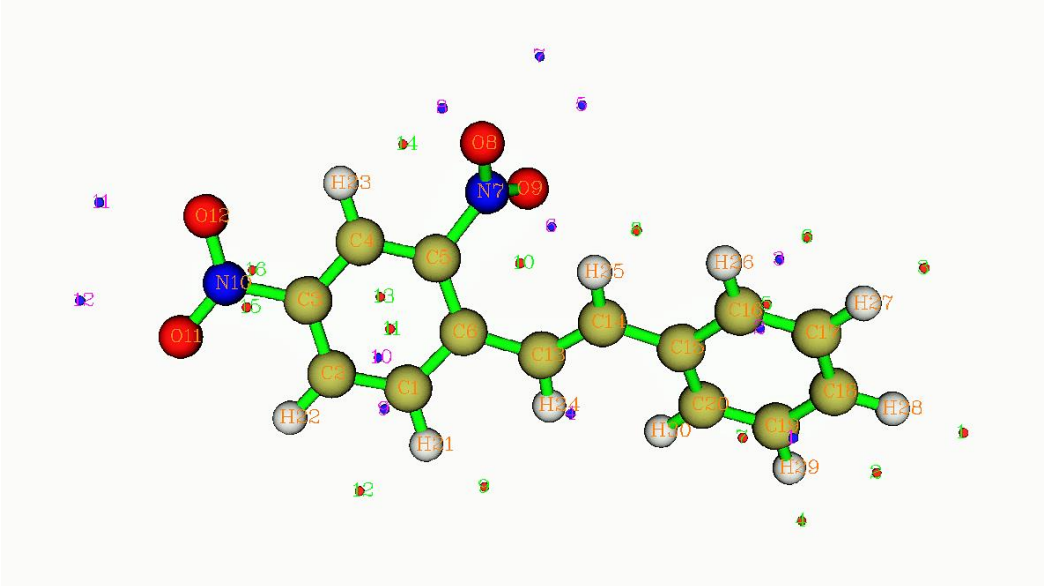


Figure S6. The distributed electrostatic potential surface maxima and surface minima of compound *trans*-1-styryl-2, 4-dinitrobenzene [B3LYP/6-311 G (d, p), 0.001 electron/b^3 isosurface], color coding: red points (electrostatic potential maximum points), blue points (electrostatic potential minimum points).

Table S7. Number of surface minima in *trans*-stilbene: 12 (* represented the minimum point)

#	a.u.	eV	kcal/mol	X/Y/Z coordinate (Angstrom)		
1	-0.0228537	-0.621879	-14.339752	-4.042363	0.137247	1.956698
2	-0.0227878	-0.620086	-14.298407	-3.881638	-0.511468	-1.960015
3	-0.0228629	-0.62213	-14.345534	-4.015336	0.157575	-1.952836
*4	-0.0228708	-0.622345	-14.350483	-3.353534	-0.768139	-1.972557
5	-0.0228596	-0.622041	-14.343481	-3.388086	-0.655273	1.949791
6	-0.0226928	-0.617502	-14.238822	-0.031033	0.031782	-2.077212
7	-0.0226717	-0.616928	-14.225587	0.048874	0.002688	2.076993
8	-0.0228649	-0.622186	-14.346831	3.404539	0.688805	-1.950087
9	-0.0228697	-0.622315	-14.349797	3.372198	0.662698	1.953042
10	-0.0228469	-0.621694	-14.335483	3.93952	-0.229682	-1.940704
11	-0.0228017	-0.620465	-14.307126	3.939201	0.297785	-1.94118
12	-0.0228615	-0.622093	-14.344687	4.023711	-0.257253	1.958865

Table S8. Number of surface maxima in *trans*-stilbene: 12: (* represented the maximum point)

#	a.u.	eV	kcal/mol	X/Y/Z Coordinate (Angstrom)		
1	0.02281784	0.620905	14.317281	-7.140894	-0.592601	0.041314
2	0.02295021	0.624507	14.400341	-5.614226	3.075451	0.021411
3	0.02297962	0.625307	14.418791	-4.698693	-3.589435	0.005994
4	-0.0207561	-0.564803	-13.023648	-3.334924	0.034931	1.763866
5	-0.0207296	-0.564081	-13.007004	-3.285827	-0.014284	-1.766277
*6	0.0289338	0.787329	18.154801	-0.578799	-2.832425	0.046144
7	0.02892247	0.78702	18.14769	0.61185	2.842063	0.03816
8	-0.0207309	-0.564117	-13.007829	3.257736	-0.016407	-1.768772
9	-0.0207607	-0.564927	-13.026511	3.282043	0.03731	1.767708
10	0.02298002	0.625318	14.419043	4.704631	3.587462	0.009199
11	0.02296854	0.625006	14.411843	5.671364	-3.034624	0.03181
12	0.02281822	0.620915	14.317519	7.142731	0.580369	0.044465

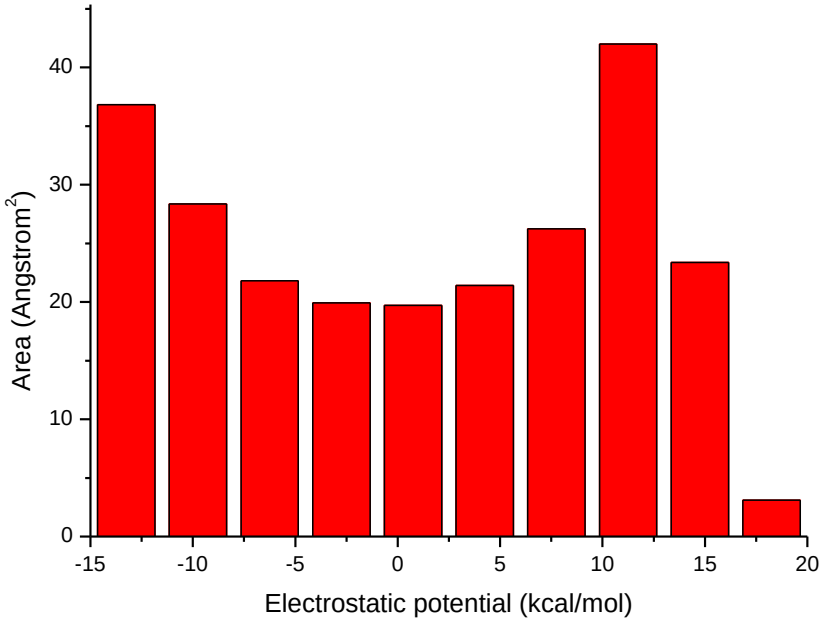


Figure S7. The electrostatic potential of compound *trans*-stilbene quantitative distribution [B3LYP/6-311+ G (d, p), 0.001 electron/b^3 isosurface].

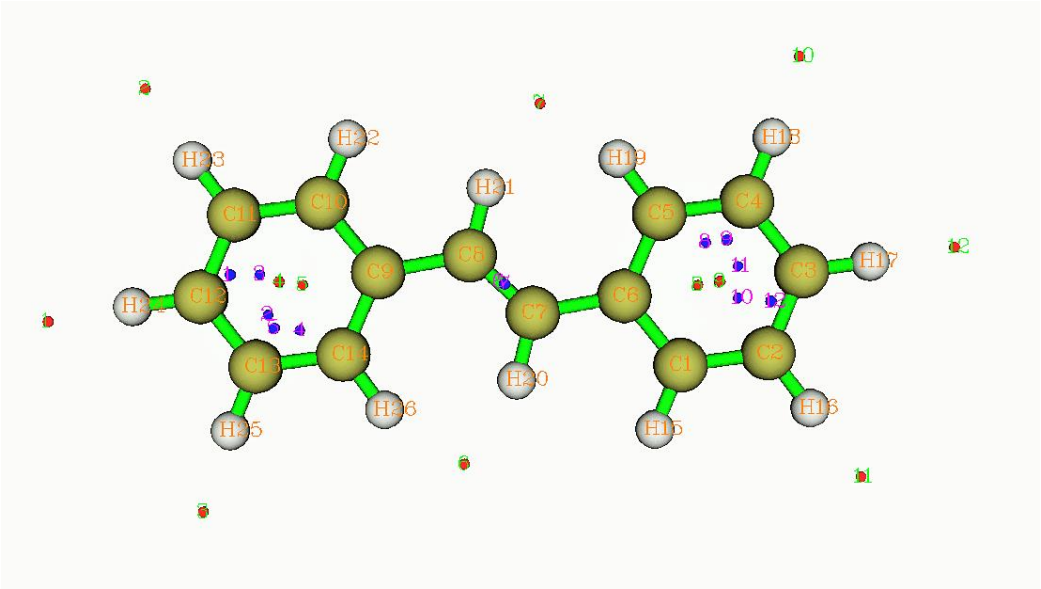
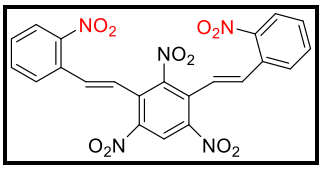
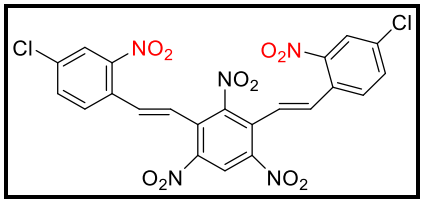


Figure S8. The distributed electrostatic potential surface maxima and surface minima of compound *trans*-stilbene [B3LYP/6-311 G (d, p), 0.001 electron/b^3 isosurface], color coding: red points (electrostatic potential maximum points), blue points (electrostatic potential minimum points).

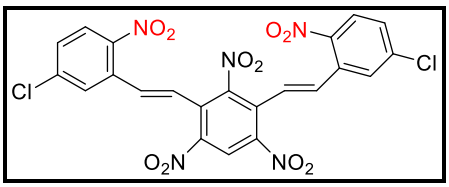
6. **Characterization Data of Synthesized Nitrostilbenes:**



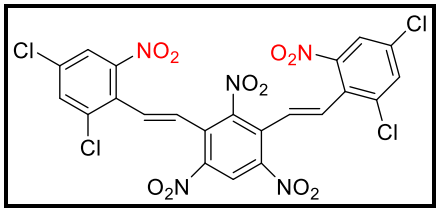
2,2'-((1*E*,1'*E*)-(2,4,6-trinitro-1,3-phenylene)bis(ethene-2,1-diyl))bis(nitrobenzene) (Table 1, entry 2a): green yellow solid, recrystallization from acetone, m.p. 212-213 ℃, IR (KBr, ν, cm^{-1}): 3097, 1629, 1603, 1550, 1524, 1341, 975; ^{1}H NMR (500 MHz, DMSO-d_6), δ 9.07 (s, 1H）8.09 (d, *J* =8.15Hz, 2H), 7.86 (d, *J* =3.95Hz, 2H), 7.68-7.66 (m, 4H), 7.50 (d, *J* =16.45Hz, 2H), 7.21 (d, *J* =16.45Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6), δ 149.76, 147.22, 146.52, 133.59, 131.02, 129.88, 129.58, 129.54, 128.32, 124.22, 122.42, 121.95. HRMS calc. for $C_{22}H_{14}N_5O_{10}$ $(M+H)^+$: 508.0210, found (M+H) 508.0206, (M+Na) 530.0121, (M+K）545.9988.



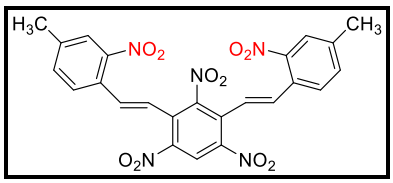
4,4'-((1E,1'E)-(2,4,6-trinitro-1,3-phenylene)bis(ethene-2,1-diyl))bis(1-chloro-3-nitrobenzene) (Table 1, entry 2b): yellow solid, recrystallization from ethanol/acetone, m.p. 249-250 ℃, IR (KBr, ν, cm^{-1}): 3083, 1630, 1599, 1584, 1550, 1527, 1381, 1344, 968; ^{1}H NMR (500 MHz, DMSO-d_6), δ 9.05 (s, 1H), 8.19 (d, *J* =2.20Hz, 2H), 7.96 (dd, J_1 =8.50Hz, J_2 =2.20Hz, 2H), 7.88 (d, *J* =8.55Hz, 2H), 7.54 (d, *J* =16.40Hz, 2H), 7.13 (d, *J* =16.40Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6), δ 149.66, 147.66, 146.54, 133.76, 133.36, 129.93, 129.83, 129.45, 128.31, 124.06, 122.63, 122.45. HRMS calc. for $C_{22}H_{12}Cl_2N_5O_{10}$ $(M+H)^+$: 574.9055, found 574.9058.



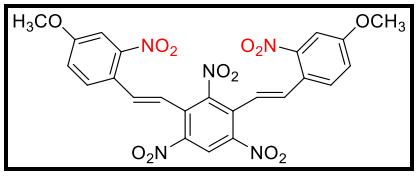
4,4'-((1E,1'E)-(2,4,6-trinitro-1,3-phenylene)bis(ethene-2,1-diyl))bis(1-chloro-3-nitrobenzene) (Table 1, entry 2c): yellow solid, recrystallization from ethanol/acetone, m.p. 207-208 ℃, IR (KBr, ν, cm^{-1}): 3010, 1602, 1521, 1468, 1390, 1342, 963; ^{1}H NMR (500 MHz, $CDCl_3$), δ 8.96 (s, 1H), 8.12 (d, *J* =8.75Hz, 2H), 7.64 (d, *J* =2.10Hz, 2H), 7.55 (dd, J_1 =8.80Hz, J_2 =2.20Hz, 2H), 7.38 (d, *J* =16.35Hz, 2H), 7.18 (d, *J* =16.35Hz, 2H); HRMS calc. for $C_{22}H_{12}Cl_2N_5O_{10}$ $(M+H)^+$: 574.9055, found 555.9052.



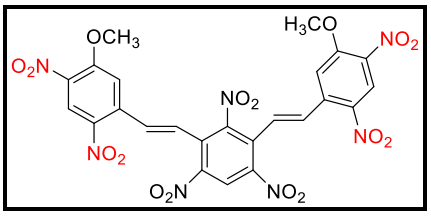
2,2'-((1E,1'E)-(2,4,6-trinitro-1,3-phenylene)bis(ethene-2,1-diyl))bis(1,5-dichloro-3-nitrobenzene) (Table 1, entry 2d): yellow solid, recrystallization from ethanol/acetone, m.p. 216-217°C, IR (KBr, ν, cm^{-1}): 3096, 1710, 1587, 1548, 1519, 1460, 1394, 1342, 958; ^{1}H NMR (500 MHz, DMSO-d_6), δ 9.06 (s, 1H), 8.41 (s, 2H), 8.12 (s, 2H), 7.70 (d, *J* =16.40Hz, 2H), 7.12 (d, *J* =16.40Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6), δ 149.49, 146.62, 145.86, 136.42, 131.90, 129.71, 129.49, 129.24, 129.10, 126.30, 123.63, 122.60. HRMS calc. for $C_{22}H_{10}Cl_4N_5O_{10}$ $(M+H)^+$: 645.9233, found 645.9235.



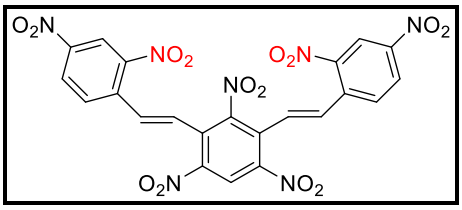
4,4'-((1E,1'E)-(2,4,6-trinitro-1,3-phenylene)bis(ethene-2,1-diyl))bis(1-methyl-3-nitrobenzene) (Table 1, entry 2e): yellow solid, recrystallization from ethanol/acetone, m.p. 239-240 ℃, IR (KBr, ν, cm^{-1}): 3083, 2926, 1630, 1577, 1542, 1526, 1376, 1345, 964; ^{1}H NMR (500 MHz, DMSO-d_6), δ 9.04 (s, 1H), 7.90 (s, 2H), 7.76 (d, *J* =8.00Hz, 2H), 7.67 (d, *J* =8.00Hz, 2H), 7.44 (d, *J* =16.45Hz, 2H), 7.15 (d, *J* =16.45Hz, 2H), 2.43 (s, 6H).



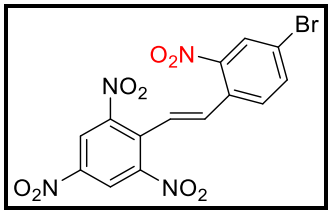
4,4'-((1E,1'E)-(2,4,6-trinitro-1,3-phenylene)bis(ethene-2,1-diyl))bis(1-methoxy-3-nitrobenzene) (Table 1, entry 2f): bright yellow solid, recrystallization from ethanol/acetone, m.p. 210-211°C, IR (KBr, ν, cm^{-1}): 3127, 3091, 2848, 1617, 1529, 1400, 1348, 1275, 975; ^{1}H NMR (500 MHz, DMSO-d_6), δ 9.02 (s, 1H), 8.20 (d, *J* =2.10Hz, 2H), 7.92 (dd, J_1 =8.85Hz, J_2 =2.15Hz, 2H), 7.48 (d, *J* =16.65Hz, 2H), 7.43 (d, *J* =8.90Hz, 2H), 6.89 (d, *J* =16.65Hz, 2H), 3.96 (s, 6H); ^{13}C NMR (126 MHz, DMSO-d_6), δ 151.96, 149.63, 146.17, 139.10, 134.11, 132.52, 129.60, 127.14, 122.91, 122.36, 117.13, 114.35, 56.47. HRMS calc. for $C_{24}H_{17}N_5O_{12}$ $(M+H)^+$: 568.0874, found 568.0877.



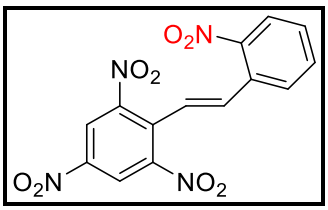
5,5'-((1E,1'E)-(2,4,6-trinitro-1,3-phenylene)bis(ethene-2,1-diyl))bis(1-methoxy-2,4-dinitrobenzene) (Table 1, entry 2g): White solid, recrystallization from *n*-hexane/acetone, m.p. 230-232 °C, IR (KBr, ν, cm^{-1}): 3093, 2950, 2855, 1610, 1590, 1552, 1527, 1398, 1343, 1300, 969; ^{1}H NMR (300 MHz, DMSO-d_6), δ 9.11 (s, 1H), 8.71 (s, 2H), 7.78 (d, *J* =16.60Hz, 2H), 7.53 (s, 2H), 7.35 (d, *J* =16.60Hz, 2H), 4.17 (s, 6H); ^{13}C NMR (75 MHz, DMSO-d_6), δ 155.67, 150.41, 147.60, 139.46, 138.11, 137.17, 131.66, 130.34, 130.18, 125.58, 123.64, 114.52, 58.22. HRMS calc. for $C_{24}H_{16}N_7O16$ $(M+H)^+$: 658.0575, found 658.0576.



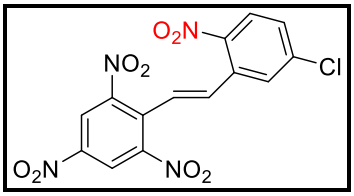
4,4'-((1E,1'E)-(2,4,6-trinitro-1,3-phenylene)bis(ethene-2,1-diyl))bis(1,3-dinitrobenzene) (Table 1, entry 2h)) Pale yellow solid, m. p. 226-227 ℃, IR (KBr, ν, cm^{-1}): 3098, 1625, 1608, 1555, 1530, 1342, 970; ^{1}H NMR (500MHz, DMSO-d_6), δ 9.10 (s, 1H), 8.79 (d, *J* =2.30Hz, 2H), 8.66-8.64 (dd, J_1 =2.30Hz, J_2 =8.65Hz, 2H), 8.11 (d, *J* =8.65Hz, 2H), 7.73 (d, *J* =16.45Hz, 2H), 7.26 (d, *J* =16.45Hz, 2H); ^{13}C NMR (126MHz, DMSO-d_6), δ 149.57, 147.00, 146.82, 146.71, 135.27, 129.95, 129.58, 129.38, 127.63, 125.33, 122.61, 119.80. HRMS calc. for $C_{22}H_{12}N_7O_{14}$ $(M+H)^+$: 597.0364, found (M+H) 597.0349, elemental analysis, calcd (%) for $C_{22}H_{11}N_7O_{14}$: C: 44.23; H: 1.86; N: 16.41; Found, C: 44.18; H: 1.82; N: 16.33.



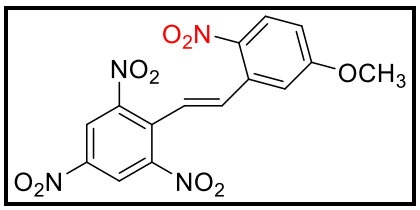
(E)-2-(4-bromo-2-nitrostyryl)-1,3,5-trinitrobenzene (Table 1, entry 2i): yellow solid, recrystallization from ethanol/acetone, m.p. 213-214 °C, IR (KBr, ν, cm^{-1}): 3101, 3081, 1632, 1598, 1552, 1534, 1473, 1401, 1342, 960; ^{1}H NMR (300 MHz, DMSO-d_6), δ 9.14 (s, 2H), 8.30 (d, *J* =2.10Hz, 1H), 8.11 (dd, J_1 =8.10Hz, J_2 =2.10Hz, 1H), 7.82 (d, *J* =8.10Hz, 1H), 7.64 (d, *J* =16.40Hz, 1H), 7.06 (d, *J* =16.40Hz, 1H). ^{13}C NMR (75 MHz, DMSO-d_6), δ 149.75, 148.48, 147.11, 137.20, 132.20, 130.81, 130.20, 129.83, 127.71, 124.29, 123.50, 122.59. HRMS calc. for $C_{14}H_8BrN_4O_8$ $(M+H)^+$: 437.9448, found (M+H) 437.9420, elemental analysis, calcd (%) for $C_{14}H_7BrN_4O_8$: C: 38.29; H: 1.61; N: 12.76; Found, C: 38.23; H: 1.66; N: 12.33.



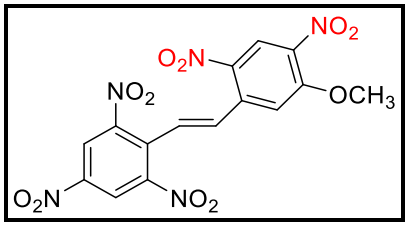
(E)-1,3,5-trinitro-2-(2-nitrostyryl)benzene [4] **(Table 1, entry 2j):** yellow solid, recrystallization from acetone, m.p. 179-180 ℃, (lit.[4] 181°C), IR (ν, cm^{-1}): 3112, 3090, 1606, 1541, 1439, 1405, 1347, 969; ^{1}H NMR (500 MHz, $CDCl_3$), δ 8.99 (s, 2H), 8.15 (d, *J* =8.20Hz, 1H), 7.75 (d, *J* =3.70Hz, 2H), 7.6-7.58 (m, 1H), 7.32 (d, *J* =16.40Hz, 1H), 7.26 (d, *J* =16.40Hz, 1H).



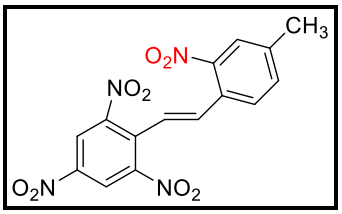
(E)-2-(5-chloro-2-nitrostyryl)-1,3,5-trinitrobenzene (Table 1, entry 2k): yellow solid, recrystallization from ethanol/acetone, m.p. 198-199°C, IR (KBr, ν, cm^{-1}): 3087, 1602, 1541, 1516, 1455, 1401, 1346, 960; ^{1}H NMR (500 MHz, $CDCl_3$), δ 9.03 (s, 2H), 8.13 (d, *J* =8.80Hz, 1H), 7.70 (d, *J* =2.20Hz, 1H), 7.56 (dd, J_1 =8.80Hz, J_2 =2.25Hz, 1H), 7.34 (d, *J* =16.40Hz, 1H), 7.20 (d, *J* =16.40Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$), δ 149.30, 145.26, 135.97, 135.52, 134.09, 132.42, 129.27, 128.97, 126.29, 124.65, 121.31, 117.12. HRMS calc. for $C_{14}H_8ClN_4O_8$ $(M+H)^+$: 394.9952, found 394.9948.



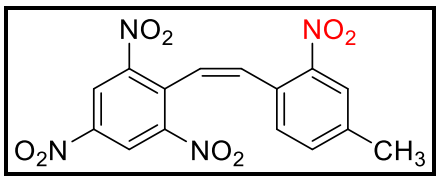
(E)-2-(5-methoxy-2-nitrostyryl)-1,3,5-trinitrobenzene (Table 1, entry 2l): yellow solid, recrystallization from ethanol/acetone, m.p. 166-167 °C, IR (KBr, ν, cm^{-1}): 3095, 2955, 2890, 2850, 1633, 1580, 1551, 1511, 1383, 1339, 972; ^{1}H NMR (500 MHz, DMSO-d_6), δ 9.14 (s, 2H), 8.17 (d, *J* =9.10Hz, 1H), 7.57 (d, *J* =16.40Hz, 1H), 7.24-7.19 (m, 3H), 3.97(s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$), δ 159.02, 150.71, 145.63, 137.95, 135.26, 130.03, 128.99, 120.68, 119.11, 115.07, 114.67, 111.71, 54.39. HRMS calc. for $C_{15}H_{11}N_4O_9$ $(M+H)^+$: 391.0448, found 391.0444.



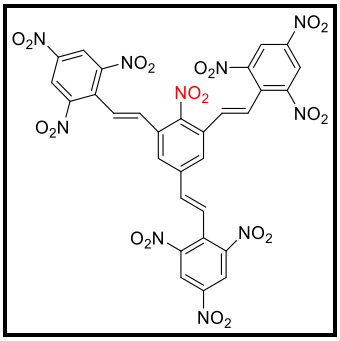
(*E*)-2-(5-methoxy-2,4-dinitrostyryl)-1,3,5-trinitrobenzene (Table 1, entry 2m): light yellow solid, recrystallization from *n*-hexane/acetone, m.p. 177-178°C, IR (KBr, ν, cm^{-1}): 3117, 3087, 3014, 2957, 2859, 1697, 1585, 1551, 1517, 1487, 1397, 1341, 1291, 972; ^{1}H NMR (300 MHz, DMSO-d_6), δ 9.15 (s, 2H), 8.70 (s, 1H), 7.84 (d, *J* =16.40Hz, 1H), 7.55 (s, 1H), 7.26 (d, *J* =16.40Hz, 1H), 4.19 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6), δ155.75, 149.77, 147.31, 139.34, 137.97, 137.49, 131.97, 130.76, 126.40, 123.67, 123.41, 114.45, 58.18. HRMS calc. for $C_{15}H_{10}N_5O_{11}$ $(M+H)^+$: 436.0299, found 436.0273; elemental analysis, calcd (%) for $C_{15}H_9N_5O_{11}$: C: 41.39; H: 2.08; N: 16.09; Found, C: 41.33; H: 2.16; N: 16.13.



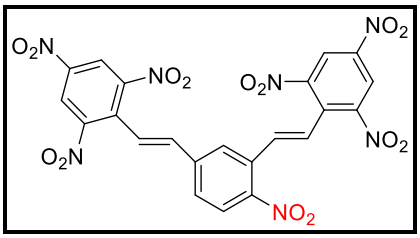
(*E*)-2-(4-methyl-2-nitrostyryl)-1,3,5-trinitrobenzene (Table 1, entry 2n, *E*-configuration): yellow solid, recrystallization from ethanol/acetone, m.p. 196-197°C, IR (KBr, ν, cm^{-1}): 3078, 1632, 1600, 1535, 1402, 1346, 969; ^{1}H NMR (300 MHz, DMSO-d_6), δ 9.11 (s, 2H), 7.89 (s, 1H), 7.76 (d, *J* =8.10Hz, 1H), 7.67 (d, *J* =8.10Hz, 1H), 7.51 (d, *J* =16.40Hz, 1H), 7.07(d, *J* =16.40Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (75 MHz, DMSO-d_6), δ 149.81, 147.87, 146.96, 141.20, 135.06, 132.38, 131.17, 128.89, 127.87, 125.14, 123.39, 122.75, 20.78. HRMS calc. for $C_{15}H_{11}N_4O_8$ $(M+H)^+$: 375.0499, found 375.0496.



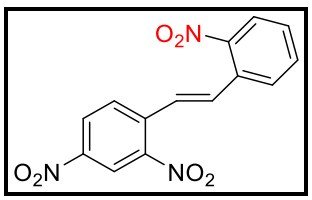
(*Z*)-2-(4-methyl-2-nitrostyryl)-1,3,5-trinitrobenzene(Table 1, entry 2n, *Z*-configuration): yellow solid, recrystallization from ethanol/acetone, m.p. 182-183°C, IR (KBr, ν, cm^{-1}): 3088, 1630, 1605, 1525, 1411, 1348, 688; ^{1}H NMR (500 MHz, DMSO-d_6), δ 8.95 (s, 2H), 8.51 (d, *J* =8.35Hz, 1H), 8.12 (s, 1H), 7.74 (d, *J* =8.40Hz, 1H), 7.39 (d, *J* =7.75Hz, 1H), 7.03 (d, *J* =7.80Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6), δ 148.17, 147.75, 147.06, 144.93, 141.94, 135.89, 135.11, 134.61, 130.50, 129.11, 128.49, 124.94, 123.51, 120.23, 19.96. HRMS calc. for $C_{15}H_{11}N_4O_8$ $(M+H)^+$: 375.0499, found 375.0495.



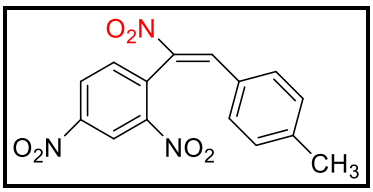
2,2',2''-((1E,1'E,1''E)-(2-nitrobenzene-1,3,5-triyl)tris(ethene-2,1-diyl))tris(1,3,5-trinitrobenzene) (Table 1, entry 2o): pale yellow solid, recrystallization from methanol/acetone, m.p. more than 280°C, IR (KBr, ν, cm^{-1}): 3097, 2883, 1604, 1541, 1402, 1346, 1271, 964; ^{1}H NMR (300 MHz, DMSO-d_6), δ 9.19 (s, 2H), 9.14 (s, 4H), 8.22 (s, 2H), 7.96-7.85 (m, 3H), 7.06 (d, *J* =16.40Hz, 1H), 6.65 (d, *J* =16.40Hz, 2H); ^{13}C NMR (75 MHz, DMSO-d_6), δ 149.85, 148.25, 147.22, 138.68, 133.86, 132.23, 128.97, 127.47, 126.47, 125.89, 123.48. HRMS calc. for $C_{30}H_{15}N_{10}O_{20}$ $(M+H)^+$: 835.0386, found 835.0352; elemental analysis, calcd (%) for $C_{30}H_{14}N_{10}O_{20}$: C: 43.18; H: 1.69; N: 16.79; Found, C: 43.23; H: 1.63; N: 16.63.



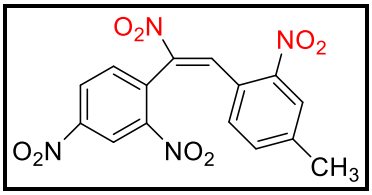
2,2'-((1E,1'E)-(4-nitro-1,3-phenylene)bis(ethene-2,1-diyl))bis(1,3,5-trinitrobenzene) (Table 1, entry 2p): pale yellow solid, recrystallization from ethanol/acetone, m.p. 124-126 °C, IR (KBr, ν, cm^{-1}): 3098, 2882, 1603, 1541, 1402, 1345, 963; ^{1}H NMR (300 MHz, DMSO-d_6), δ 9.16 (s, 2H), 9.14 (s, 2H), 8.16 (d, *J* =8.10Hz, 1H), 7.98-7.91 (m, 2H), 7.85 (d, *J* =16.40Hz, 1H), 7.69 (d, *J* =16.40Hz, 1H), 7.16 (d, *J* =16.50Hz, 1H), 7.02 (d, *J* =16.50Hz, 1H); ^{13}C NMR (75 MHz, DMSO-d_6), δ 149.84, 147.61, 147.38, 147.12, 146.69, 140.76, 140.43, 133.77, 132.44, 132.32, 131.52, 131.11, 128.20, 128.06, 126.15, 124.01, 123.73, 123.50. HRMS calc. for $C_{22}H_{12}N_7O_{14}$ $(M+H)^+$: 598.0364, found 598.0358.



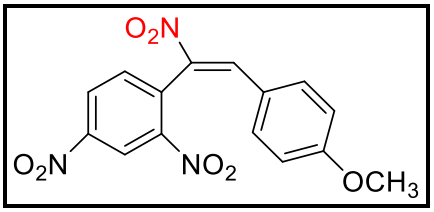
(E)-2,4-dinitro-1-(2-nitrostyryl)benzene (Table 2, entry 3a): yellow solid, recrystallization from ethanol/acetone, m.p. 195-196 °C, IR (ν, cm^{-1}): 3106, 1629, 1605, 1571, 1517, 1443, 1346, 1262, 973; ^{1}H NMR (500 MHz, $CDCl_3$), δ 8.91 (d, *J* =2.30Hz, 1H), 8.52 (dd, J_1 =8.65Hz, J_2 =2.25Hz, 1H), 8.12 (d, *J* =8.25Hz, 1H), 8.05 (d, *J* =8.65Hz, 1H), 7.82 (d, *J* =7.55Hz, 1H), 7.78 (d, *J* =16.05Hz, 1H), 7.73 (d, *J* =7.65Hz, 1H), 7.58-7.55 (m, 2H).



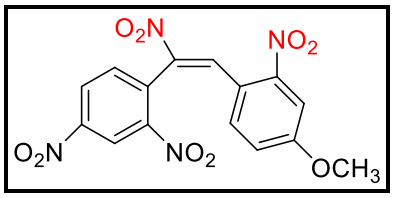
(*E*)-2,4-dinitro-1-(1-nitro-2-(p-tolyl)vinyl)benzene (Table 2, entry 3b): yellow solid, pure nitrated product was isolated by column chromatography through a silica gel column (mesh 100–200). Eluent: ethyl acetate/ *n*-hexane (1:20 v/v). m.p. 224-225 °C, IR (KBr, ν, cm^{-1}): 3087, 2924, 2858, 1603, 1515, 1347, 815; ^{1}H NMR (300 MHz, $CDCl_3$), δ 8.89 (s, 1H), 8.50 (d, *J* =8.55Hz, 1H), 8.05 (d, *J* =8.55Hz, 1H), 7.91 (s, 1H), 7.71 (d, *J* =8.20Hz, 2H), 7.57 (d, *J* =8.20Hz, 2H), 2.50 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$), δ 149.20, 144.69, 139.68, 138.41, 133.10, 132.88, 131.14, 128.74, 126.54, 121.13, 114.09, 20.45. HRMS calc. for $C_{15}H_{12}N_3O_6$ $(M+H)^+$: 330.0648, found 330.0645.



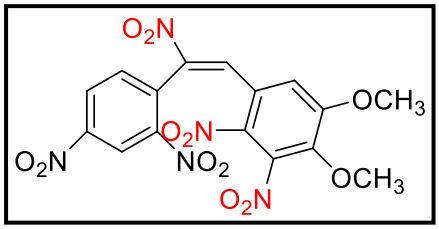
(*E*)-1-(2-(2,4-dinitrophenyl)-2-nitrovinyl)-4-methyl-2-nitrobenzene (Table 2, entry 3c): yellow solid, pure nitrated product was isolated by column chromatography through a silica gel column (mesh 100–200). Eluent: ethyl acetate/ *n*-hexane (1:20 v/v). m.p. 198-199 ℃, IR (KBr, ν, cm^{-1}): 3106, 3062, 2925, 2867, 1657, 1599, 1521, 1347, 806. ^{1}H NMR (300 MHz, $CDCl_3$), δ 9.11 (d, *J* =2.10Hz, 1H), 8.71 (s, 1H), 8.37 (dd, J_1 =8.15Hz, J_2 =2.10Hz, 1H), 8.06 (s, 1H), 7.43 (d, *J* =8.20Hz, 1H), 7.28 (d, *J* =8.15Hz, 1H), 6.87 (d, *J* =8.20Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$), δ 148.17, 147.75, 147.06, 144.93, 141.94, 135.89, 135.11, 134.61, 130.50, 129.11, 128.49, 124.94, 123.51, 120.23, 19.96. HRMS calc. for $C_{15}H_{11}N_4O_8$ $(M+H)^+$: 375.0599, found 375.0560.



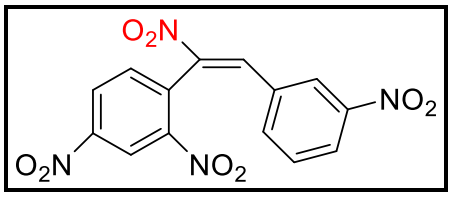
(*E*)-1-(2-(4-methoxyphenyl)-1-nitrovinyl)-2,4-dinitrobenzene (Table 2, entry 3d): Light yellow solid, pure nitrated product was isolated by column chromatography through a silica gel column (mesh 100–200). Eluent: ethyl acetate/ *n*-hexane (1:15 v/v). m.p. 172-173 °C, IR (KBr, ν, cm^{-1}): 3100, 2976, 2842, 1634, 1599, 1538, 1512, 1345, 1303,1260, 835; ^{1}H NMR (300 MHz, $CDCl_3$), δ 9.18 (s, 1H), 8.55 (d, *J* =8.40Hz, 1H), 8.40 (s, 1H), 7.65 (d, *J* =8.40Hz, 1H), 7.01 (d, *J* =8.10 Hz, 2H), 6.81 (d, *J* =8.10 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.62, 159.17, 148.81, 139.41, 136.71, 136.01, 134.88, 133.12, 128.52, 121.85, 121.04, 114.93, 55.45. HRMS calc. for $C_{15}H_{12}N_3O_7$ $(M+H)^+$: 346.0597, found 346.0597.



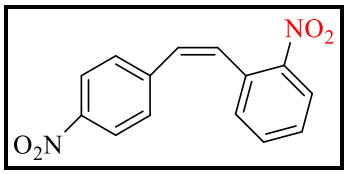
(*E*)-1-(2-(2,4-dinitrophenyl)-2-nitrovinyl)-4-methoxy-2-nitrobenzene (Table 2, entry 3e): yellow solid, pure nitrated product was isolated by column chromatography through a silica gel column (mesh 100–200). Eluent: ethyl acetate/ *n*-hexane (1:15 v/v). m.p. 177-179 °C, IR (KBr, ν, cm^{-1}): 3108, 2985, 2950, 1649, 1526, 1347, 1280, 836; ^{1}H NMR (300 MHz, DMSO-d_6), δ 9.06 (d, J =2.10 Hz, 1H), 8.73 (dd, J_1 =8.40Hz, J_2 =2.20Hz, 1H), 8.63 (s, 1H), 7.97-7.93 (t, J =5.40 Hz, 2H), 7.35 (dd, J_1 =8.90Hz, J_2 =2.10Hz, 1H), 7.25 (d, J =9.00Hz, 1H), 3.91 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 154.38, 149.31, 148.42, 144.28, 139.63, 136.83, 135.65, 135.42, 131.02, 130.01, 128.97, 122.50, 121.66, 115.40, 57.51. HRMS calc. for $C_{15}H_{11}N_4O_9$ $(M+H)^+$: 391.0450, found 391.0446.



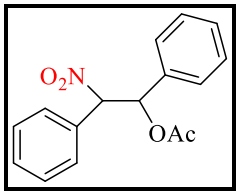
(*E*)-1-(2-(2,4-dinitrophenyl)-2-nitrovinyl)-4,5-dimethoxy-2,3-dinitrobenzene (Table 2, entry 3f): Light yellow solid, pure nitrated product was isolated by recrystallization from ethyl acetate/ *n*-hexane. m.p. 214-215 °C, IR (KBr, ν, cm^{-1}): 3108, 2993, 2945, 1656, 1563, 1532, 1345, 1306, 1256, 817; ^{1}H NMR (300 MHz, DMSO-d_6), δ 8.91 (d, J =2.00 Hz, 1H), 8.85 (s, 1H), 8.61 (dd, J_1 =8.30Hz, J_2 =2.00Hz, 1H), 7.99 (d, J =8.30Hz, 1H), 6.82 (s, 1H), 3.87 (s, 3H), 3.69 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 157.33, 149.40, 148.54, 146.90, 141.83, 140.42, 136.13, 135.07, 132.24, 129.51, 128.84, 125.42, 121.11, 115.17, 63.01, 58.00. HRMS calc. for $C_{16}H_{12}N_5O_{12}$ $(M+H)^+$: 466.0404, found 466.0401.



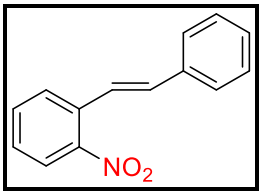
(*E*)-2, 4-dinitro-1-(1-nitro-2-(3-nitrophenyl)vinyl)benzene [5]**(Table 2, entry 3g):** Brown yellow solid, pure nitrated product was isolated by recrystallization from acetone. m.p. 200-201 ℃, IR (KBr, ν, cm^{-1}): 3101, 2983 , 1659, 1603, 1332, 819; ^{1}H NMR (300 MHz, DMSO-d_6), δ 8.99 (d, J =2.00 Hz, 1H), 8.72 (dd, J_1 =8.50Hz, J_2 =2.00Hz, 1H), 8.43 (d, J =8.50 Hz, 1H), 8.46 (s, 1H), 7.40 (d, J =2.20 Hz, 1H), 7.28-7.25 (m, 3H).



(*Z*)-1-nitro-2-(4-nitrostyryl)benzene (Table 2, entry 3h): Light yellow solid, pure nitrated product was isolated by column chromatography through a silica gel column (mesh 100–200). Eluent: ethyl acetate/ *n*-hexane (1:10 v/v). m.p. 188-189 °C, IR (KBr, ν, cm^{-1}): 3108, 1654, 1600, 1520, 1347, 1323, 687; ^{1}H NMR (300 MHz, $CDCl_3$), δ 8.15 (d, *J* =8.70 Hz, 1H), 7.53 (d, *J* =8.70 Hz, 1H), 7.24-7.15 (m, 4H), 6.58 (d, *J* =10.75Hz, 1H), 5.92 (d, *J* =10.75Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.72, 138.15, 135.29, 131.29, 130.74, 128.59, 127.90, 127.58, 125.89, 125.09, 121.03, 119.90. HRMS calc. for $C_{14}H_{11}N_2O_4$ $(M+H)^+$: 271.0641, found 271.0644.

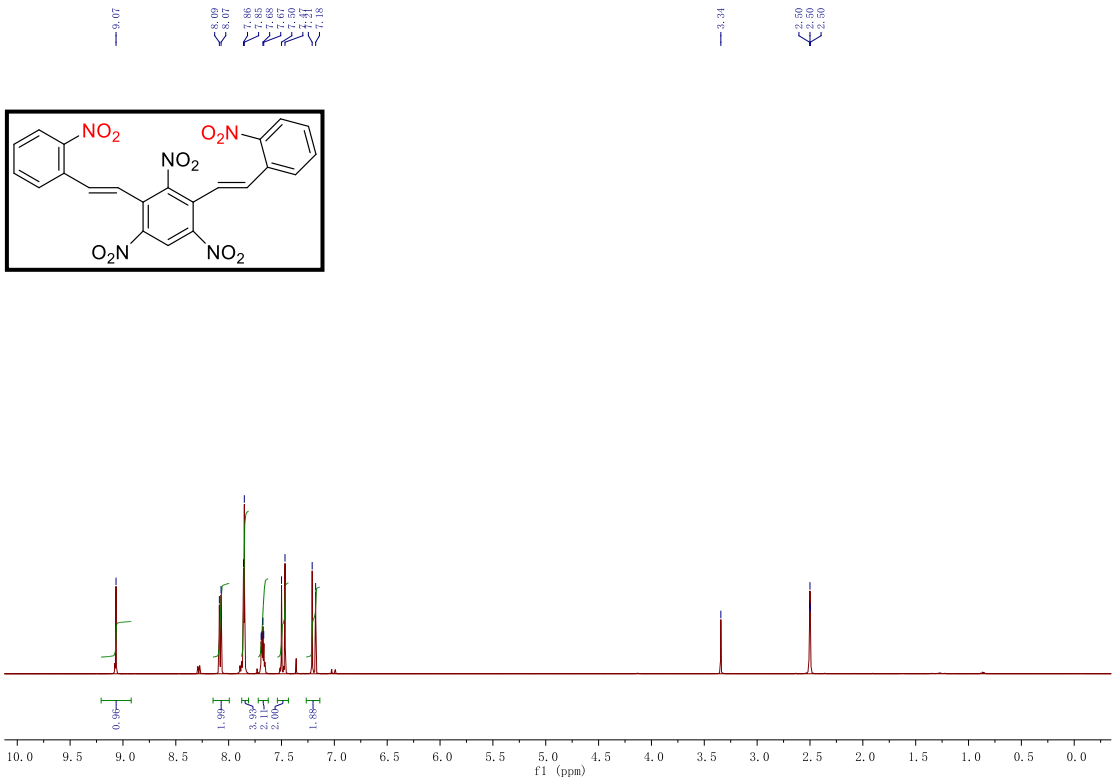


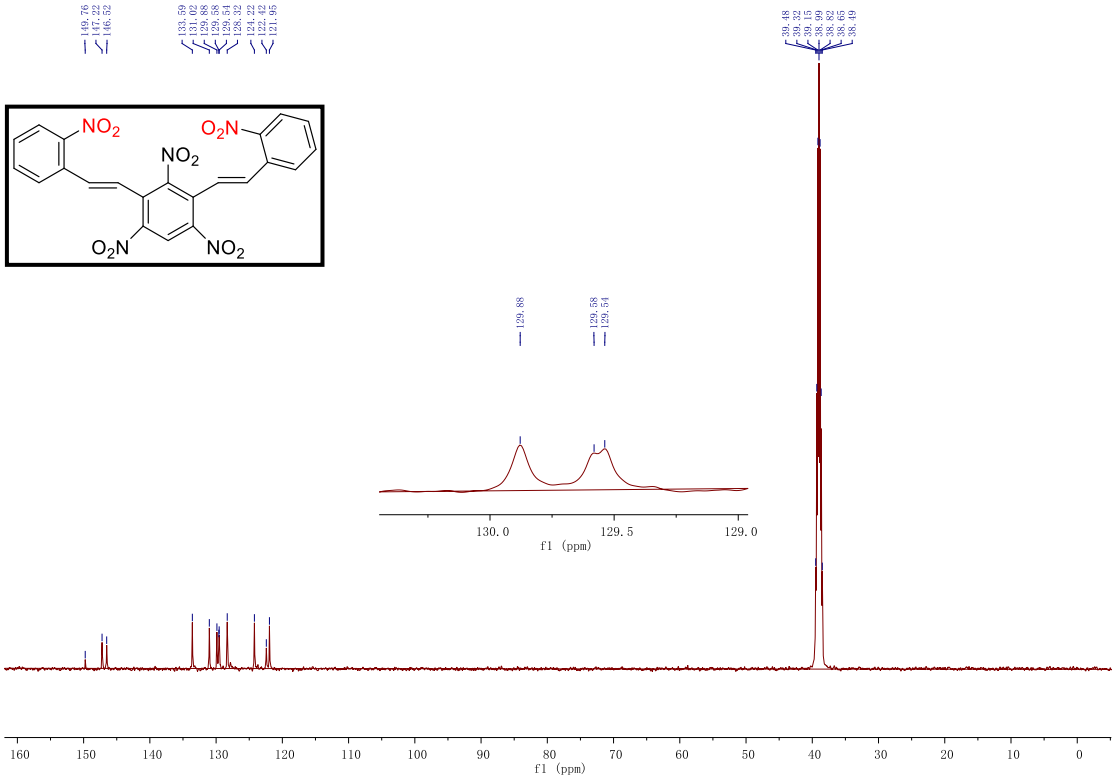
2-Nitro-1,2-diphenylethyl acetate (Table 2, entry 3i): Light yellow solid, pure nitrated product was isolated by column chromatography through a silica gel column (mesh 100–200). Eluent: ethyl acetate/ *n*-hexane (1:14 v/v). IR (KBr, ν, cm^{-1}): 3109, 1745, 1557, 1368, 1223, 1018, 723, 699; ^{1}H NMR (300 MHz, $CDCl_3$), δ 7.34-7.28 (m, 5H), 7.21-7.16 (m, 5H), 6.62 (d, *J* =10.15Hz, 1H), 5.81 (d, *J* =10.15Hz, 1H), 2.07 (s, 3H).

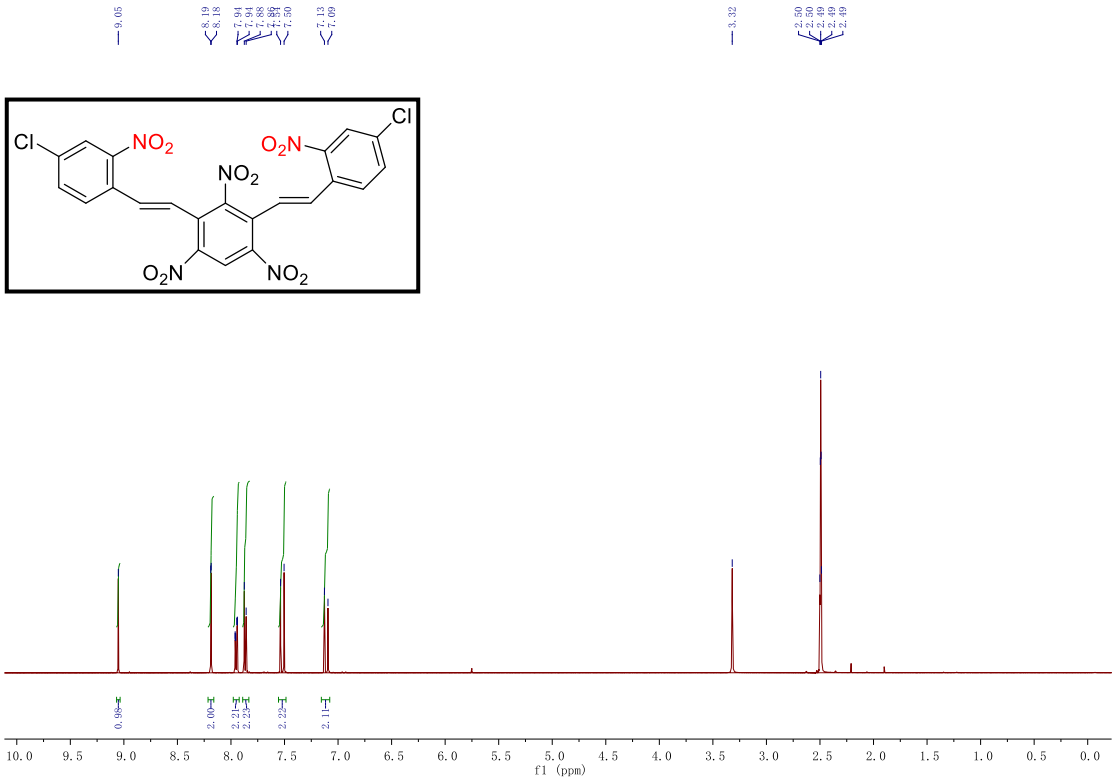


(*E*)-1-nitro-2-styrylbenzene (Table 2, entry 3j): Pale yellow solid, pure nitrated product was isolated by column chromatography through a silica gel column (mesh 100–200). Eluent: ethyl acetate/ *n*-hexane (1:14 v/v). IR (KBr, ν, cm^{-1}): 3111, 1646, 1559, 1345, 1218, 969; ^{1}H NMR (300 MHz, $CDCl_3$), δ 7.97 (d, *J* =2.15Hz, 1H), 7.77 (d, *J* =2.15Hz, 1H), 7.63-7.55 (m, 4H), 7.42-7.33 (m, 4H), 7.12 (d, *J* =16.00Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.02, 135.53, 132.89, 132.16, 132.03, 17.87, 127.67, 127.20, 127.02, 126.15, 123.80, 122.51.

7. Copies of Copies of ^{1}H and ^{13}C NMR Spectra



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2.50
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2.49
2.49
Cl
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O2N
Cl
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O2N
NO2
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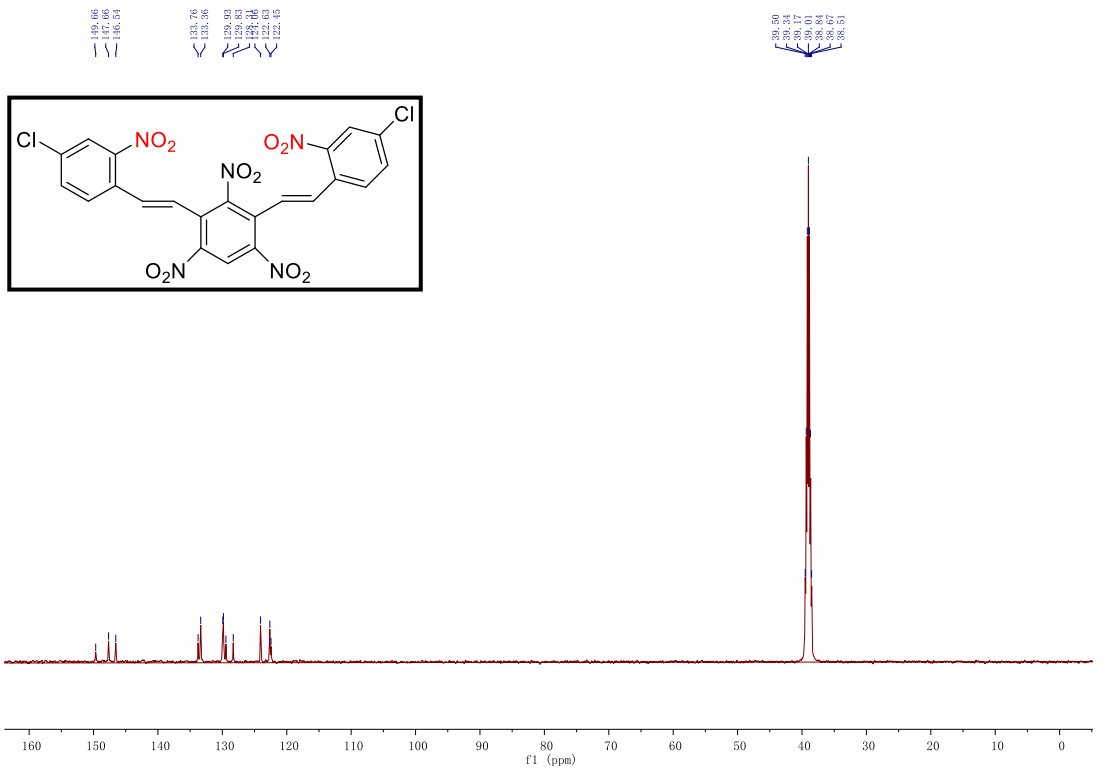
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Cl
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Cl
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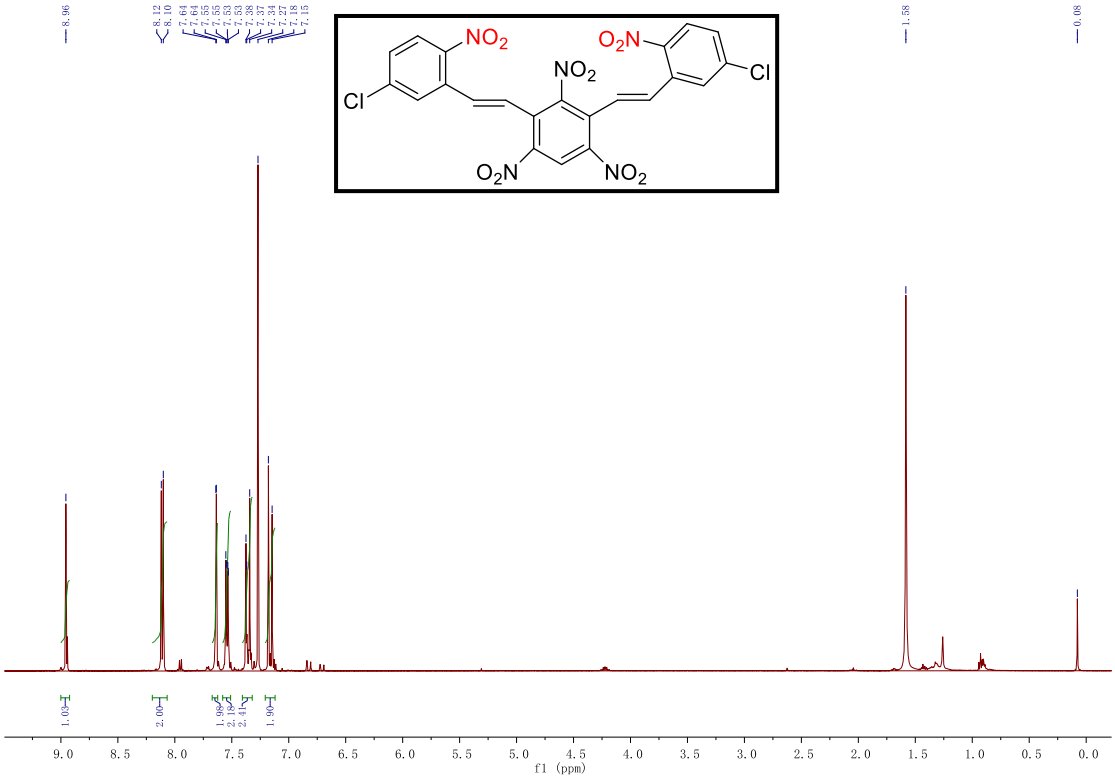
O2N
NO2
f1 (ppm)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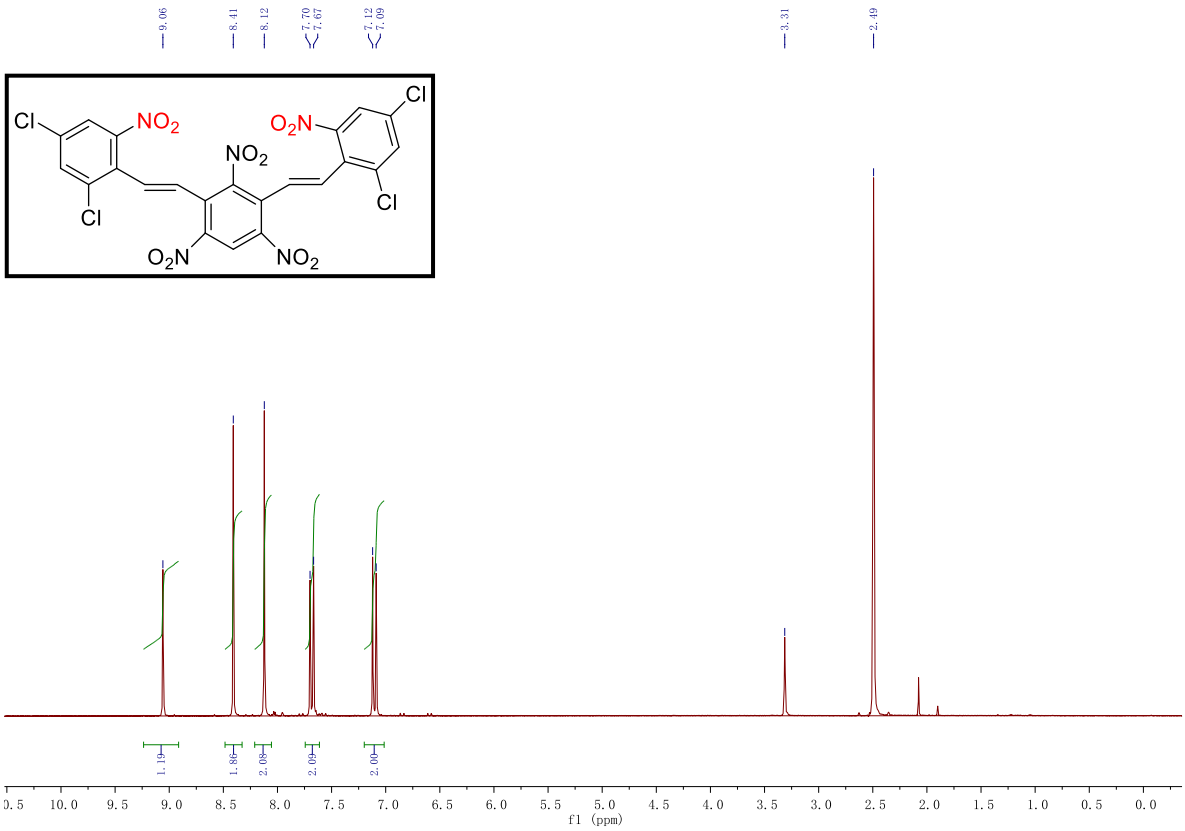
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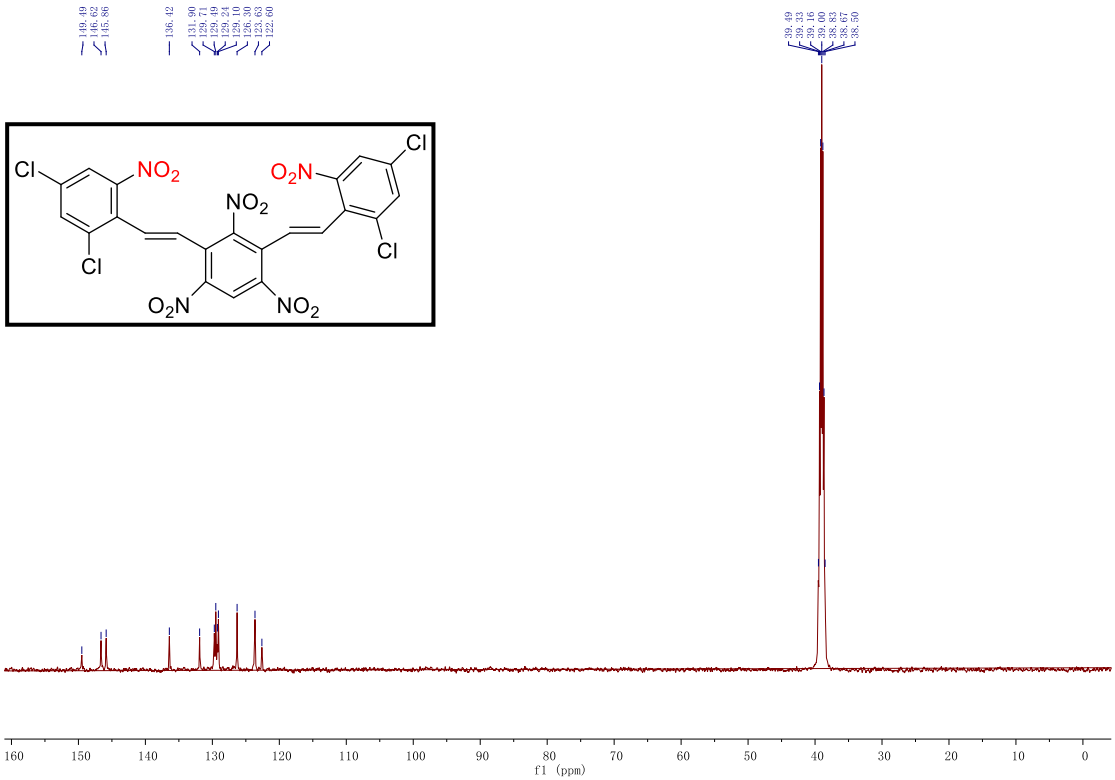
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Cl
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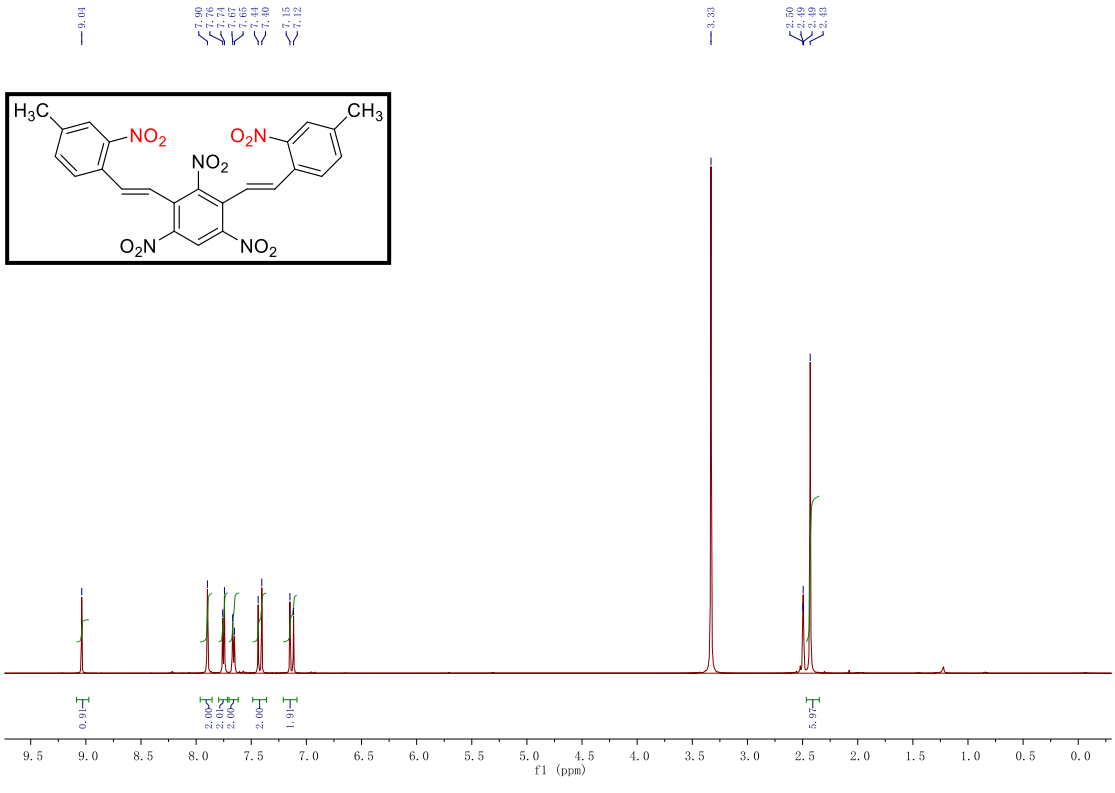
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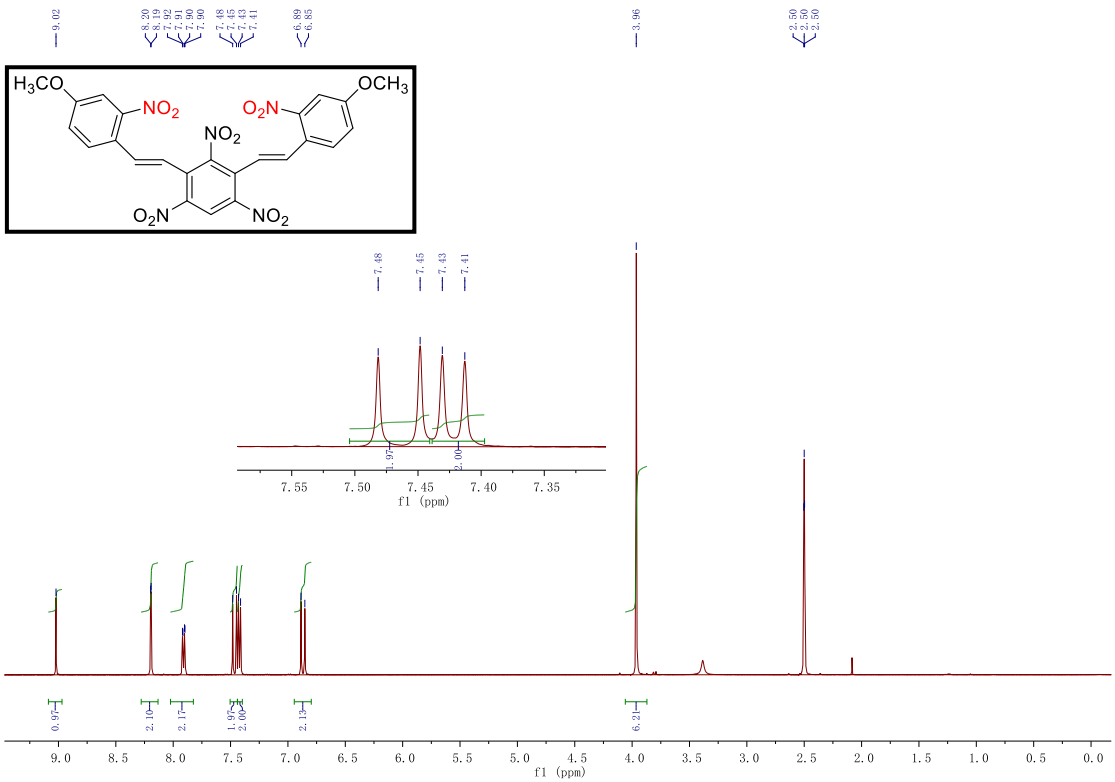
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NO2
O2N
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7.45
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7.45
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7.35
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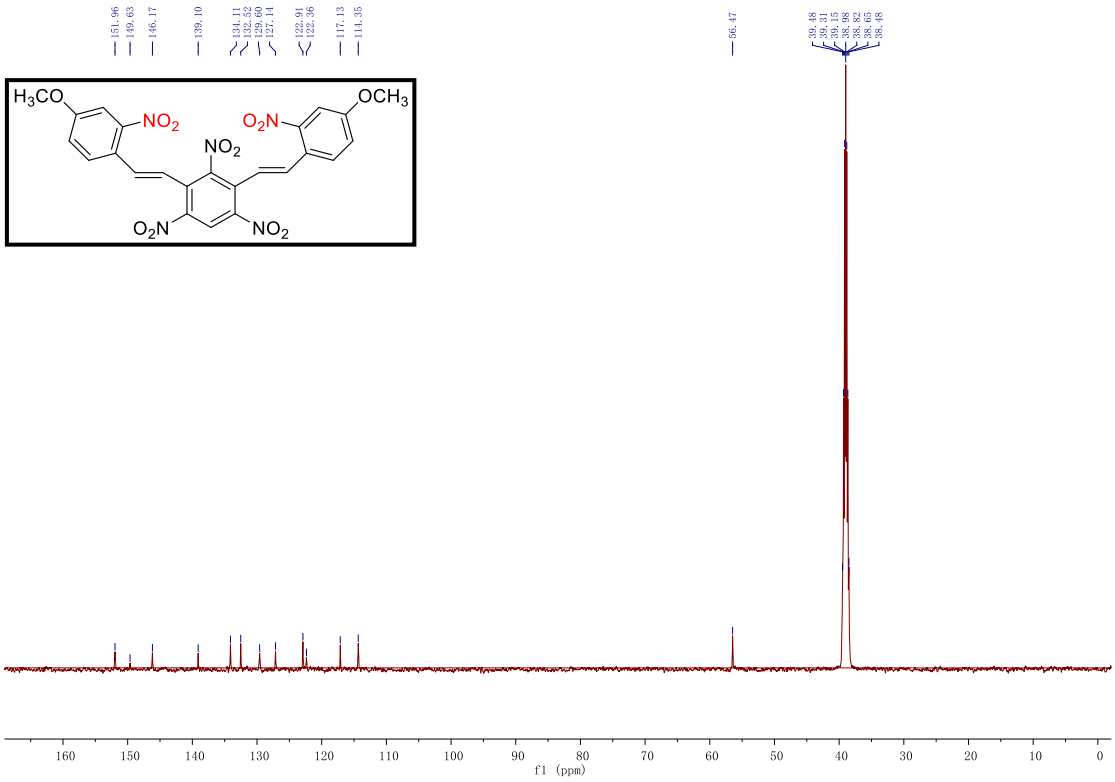
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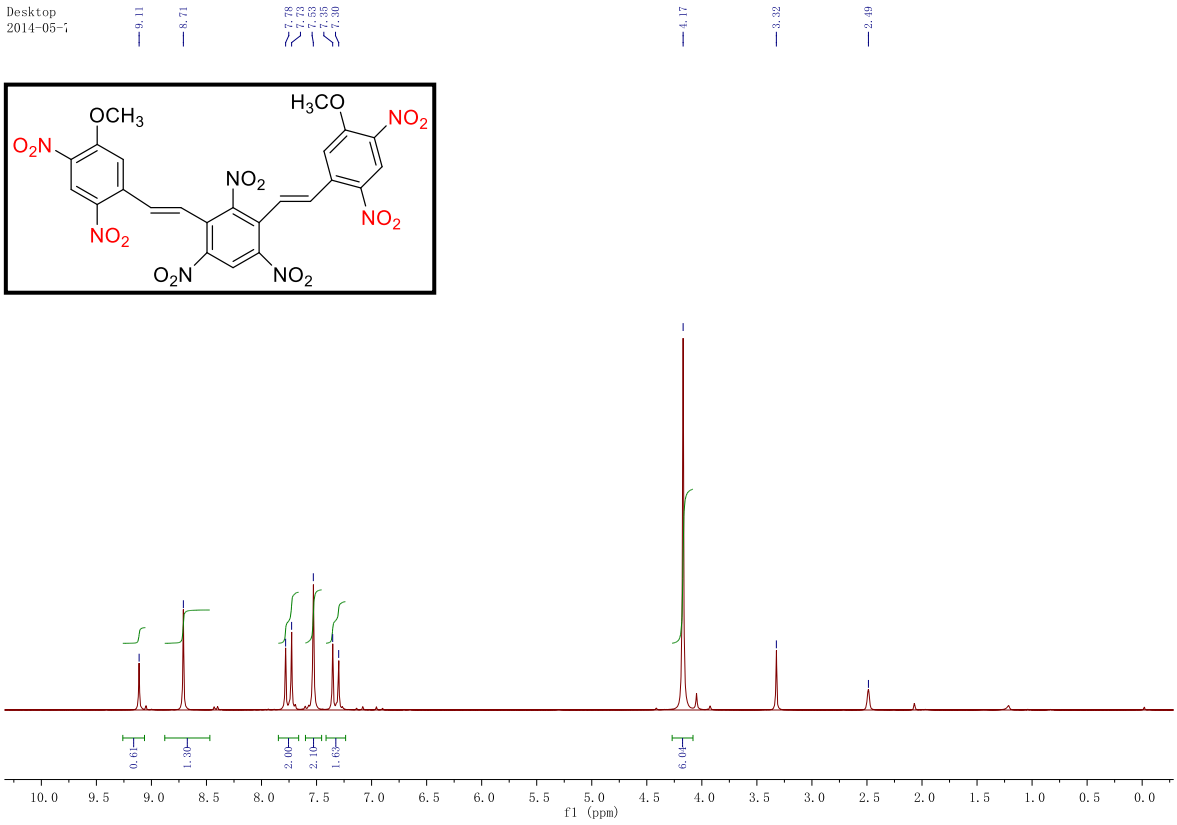
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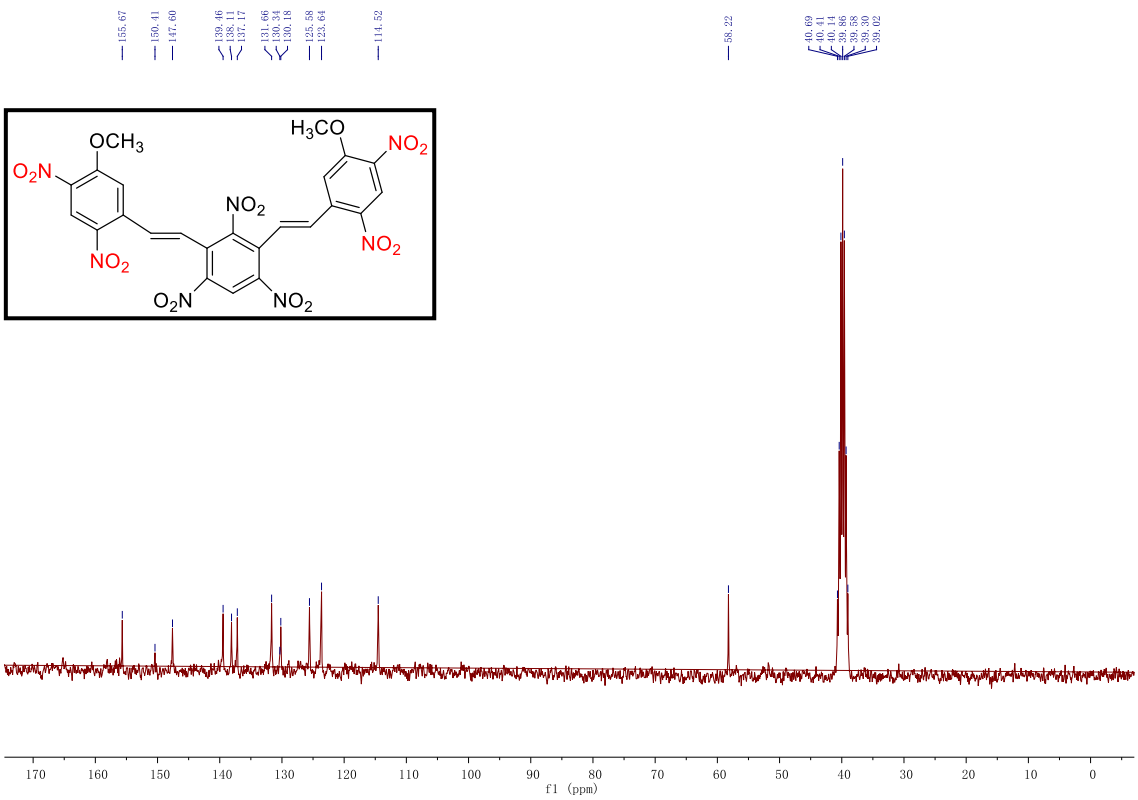
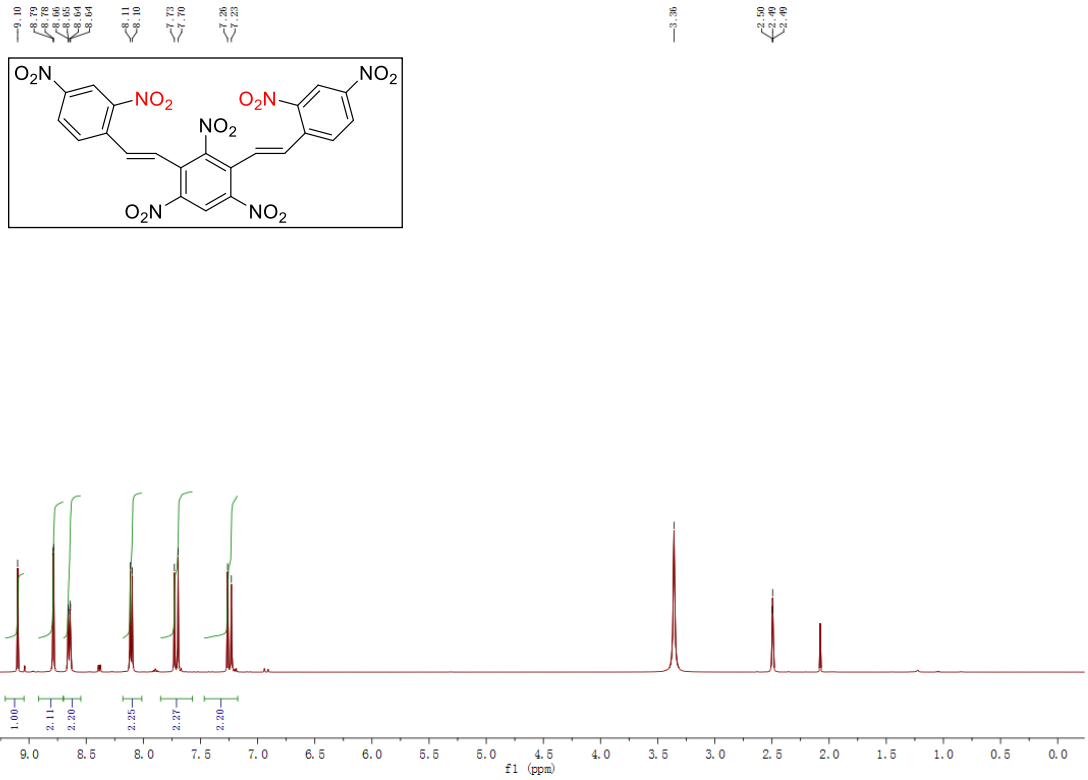
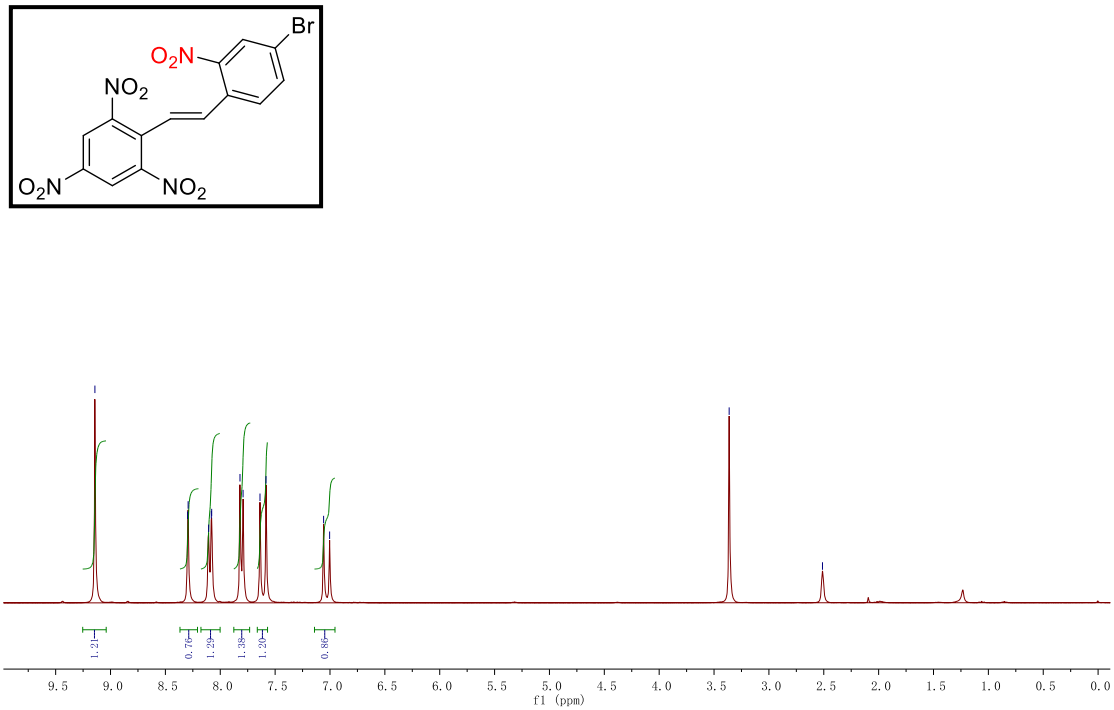
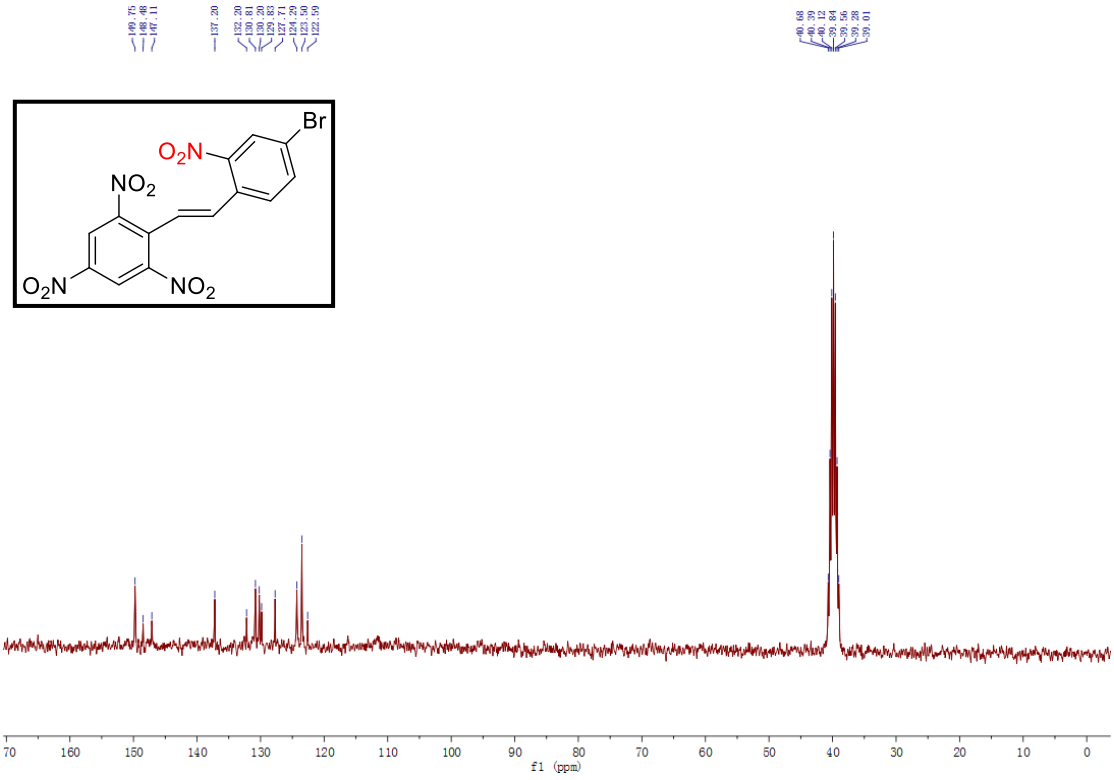
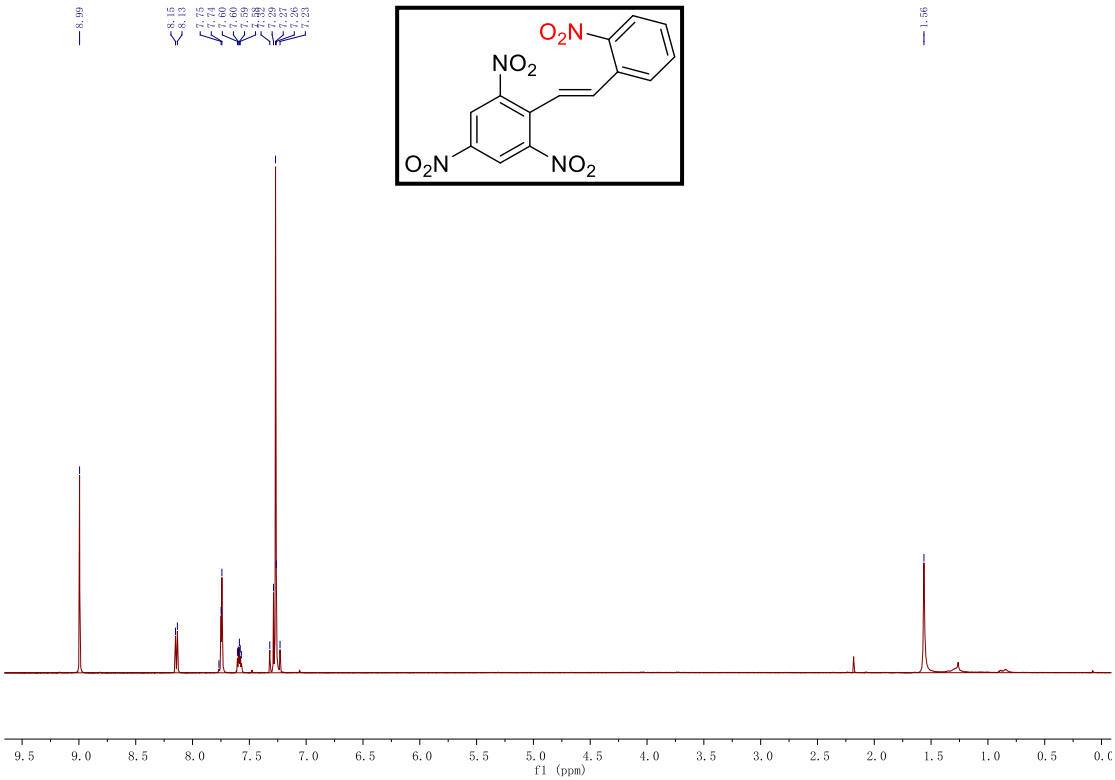
9.11
8.71
7.78
7.73
7.53
7.35
7.30
4.17
3.32
2.49
OCH3
H3CO
O2N
NO2
NO2
NO2
NO2
O2N
NO2
0.61
1.50
2.00
2.10
1.63
6.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

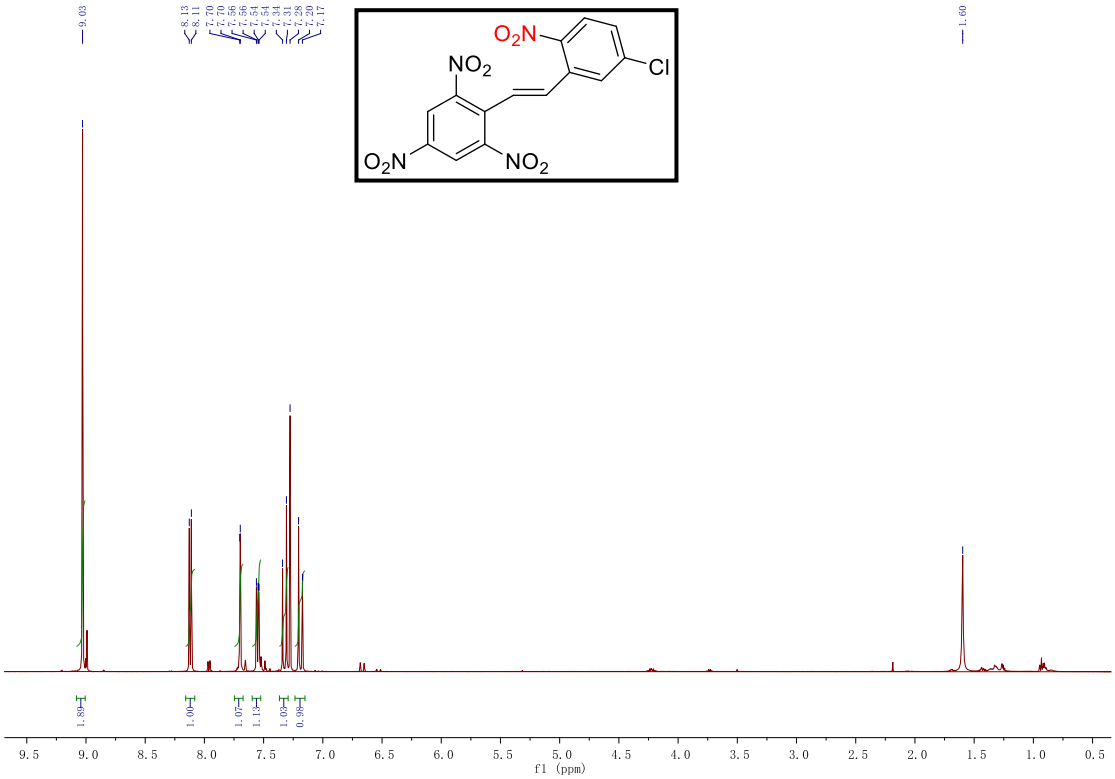

155.67
150.41
147.60
139.46
138.11
137.17
131.66
130.34
130.18
125.58
123.64
114.52
58.22
40.69
40.41
40.14
39.86
39.58
39.30
39.02
OCH3
H3CO
O2N
NO2
NO2
NO2
NO2
O2N
NO2
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

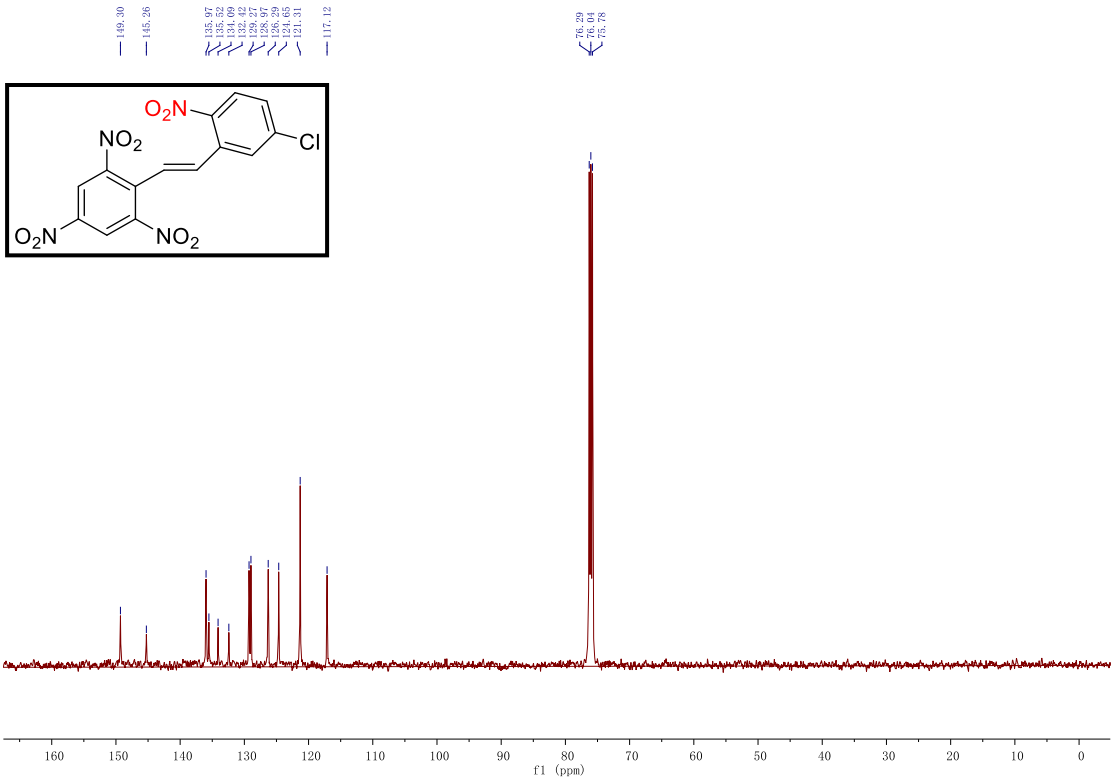


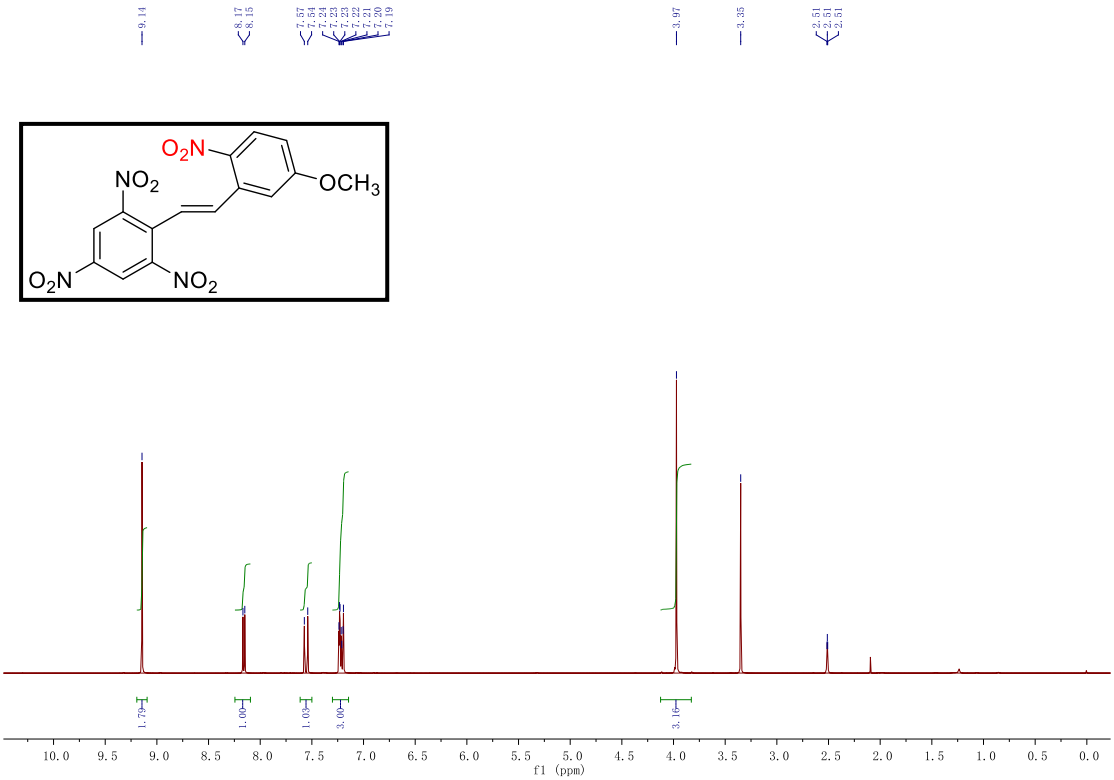

9.14
8.30
8.29
8.11
8.08
8.08
7.82
7.79
7.64
7.58
7.06
7.00
3.36
2.51
Br
O2N
NO2
O2N
NO2
1.21
0.76
1.29
1.38
1.20
0.80
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

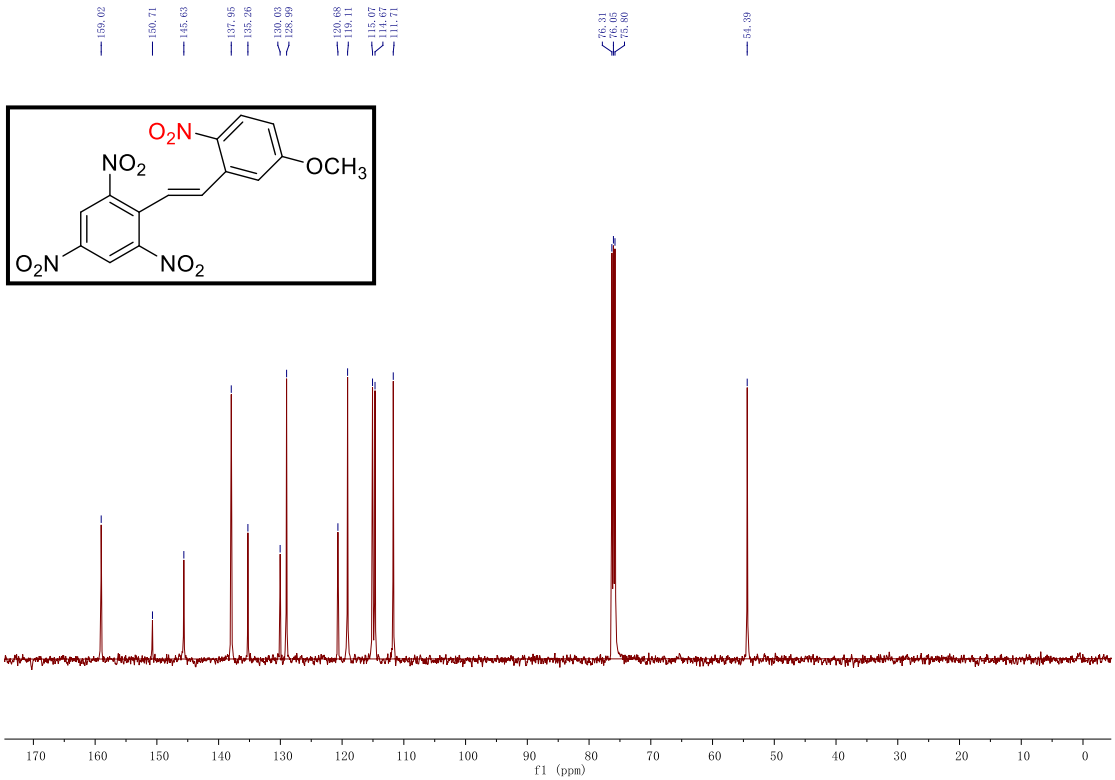

149.75
148.48
147.11
137.20
132.20
130.81
130.20
129.83
127.71
124.79
123.50
122.59
40.68
40.47
40.12
39.84
39.56
39.28
39.01
Br
O2N
NO2
O2N
NO2
70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

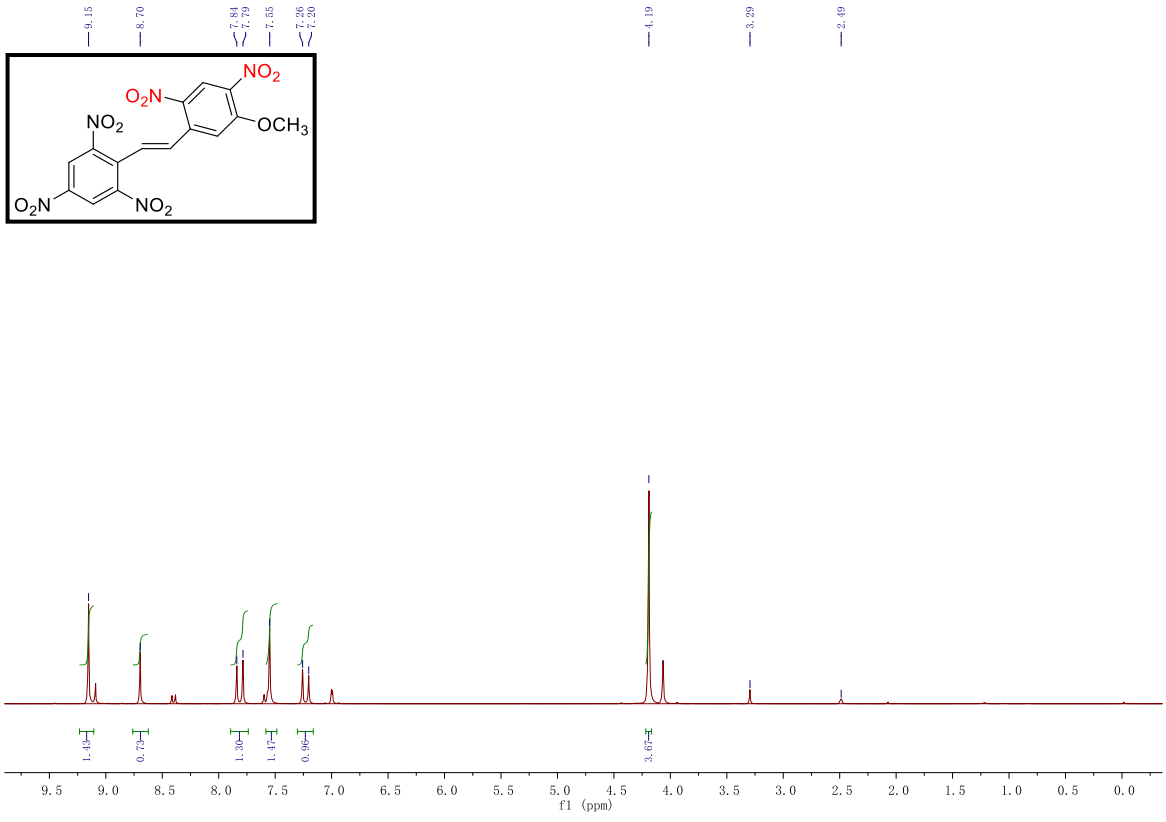

8.99
8.15
8.13
7.75
7.74
7.60
7.60
7.59
7.59
7.32
7.29
7.27
7.26
7.23
1.56
O2N
NO2
O2N
NO2
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

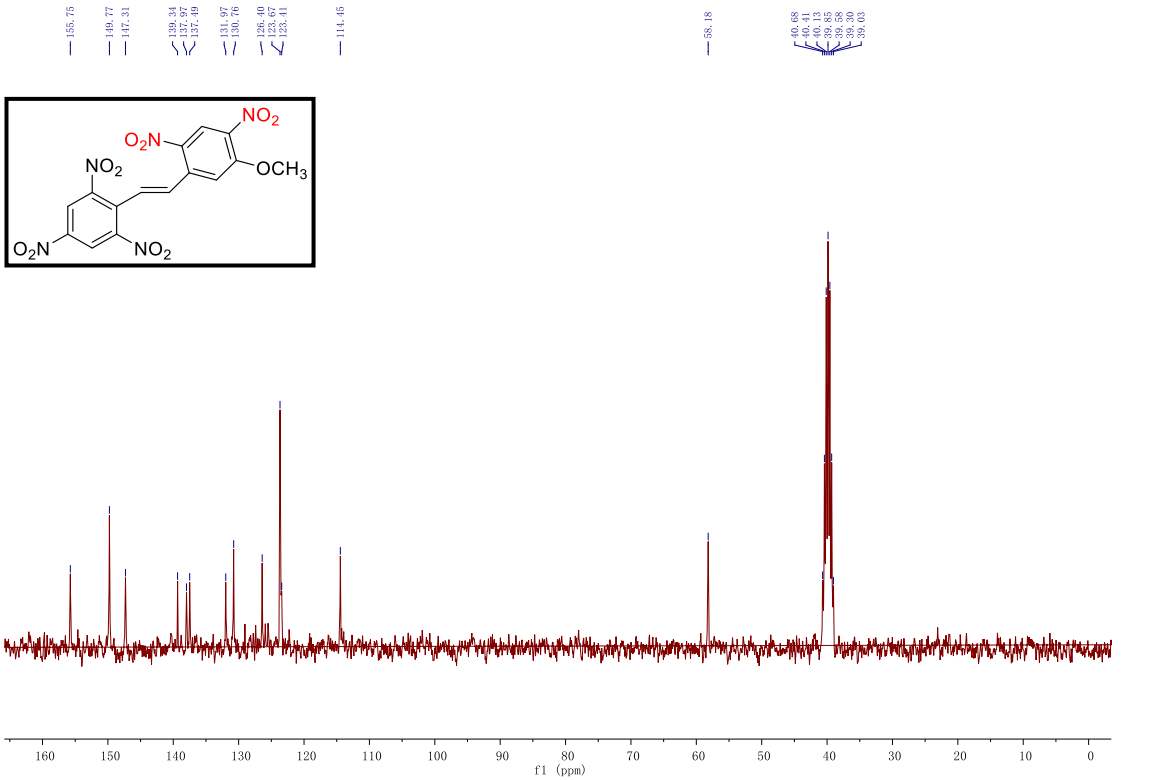

9.03
8.13
8.11
7.70
7.70
7.56
7.56
7.54
7.54
7.34
7.31
7.28
7.20
7.17
1.60
O2N
NO2
Cl
O2N
NO2
1.89
1.00
1.07
1.13
1.03
0.98
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

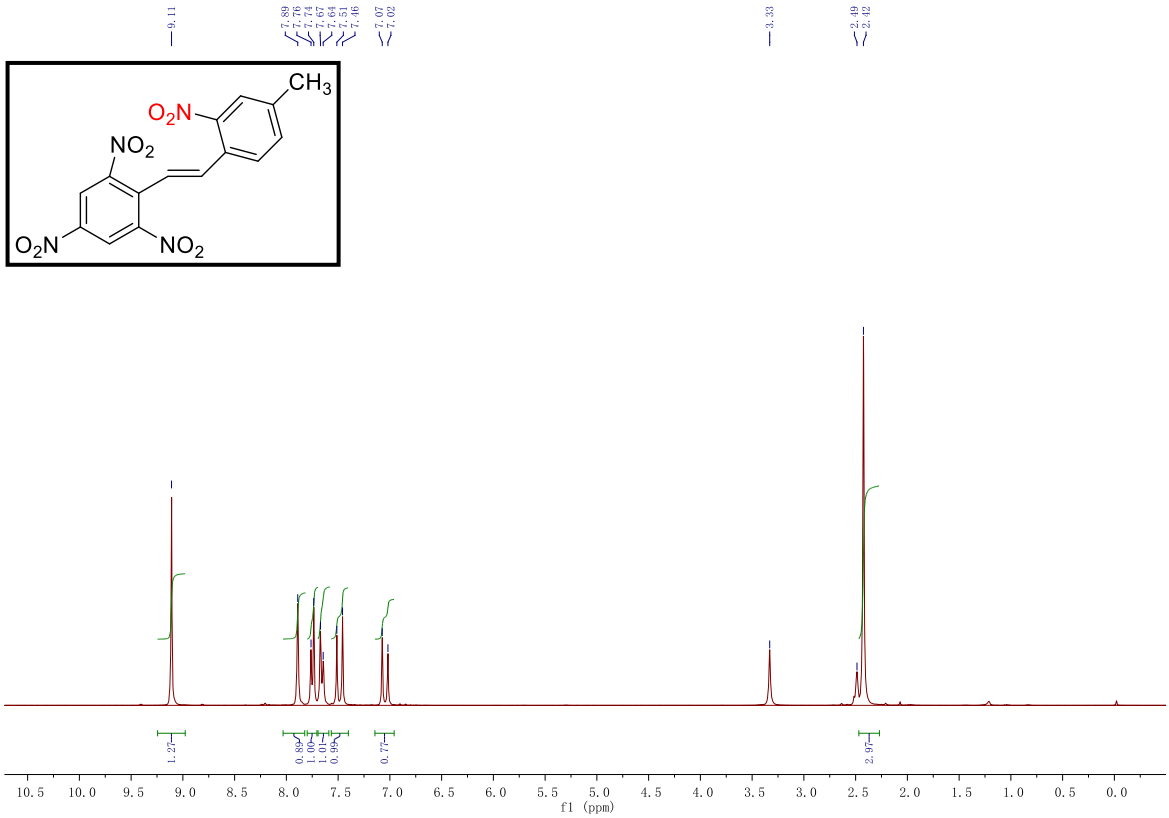

149.30
145.26
135.97
135.52
134.09
132.42
129.27
128.97
126.29
124.65
121.31
117.12
76.29
76.04
75.78
O2N
NO2
Cl
O2N
NO2
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

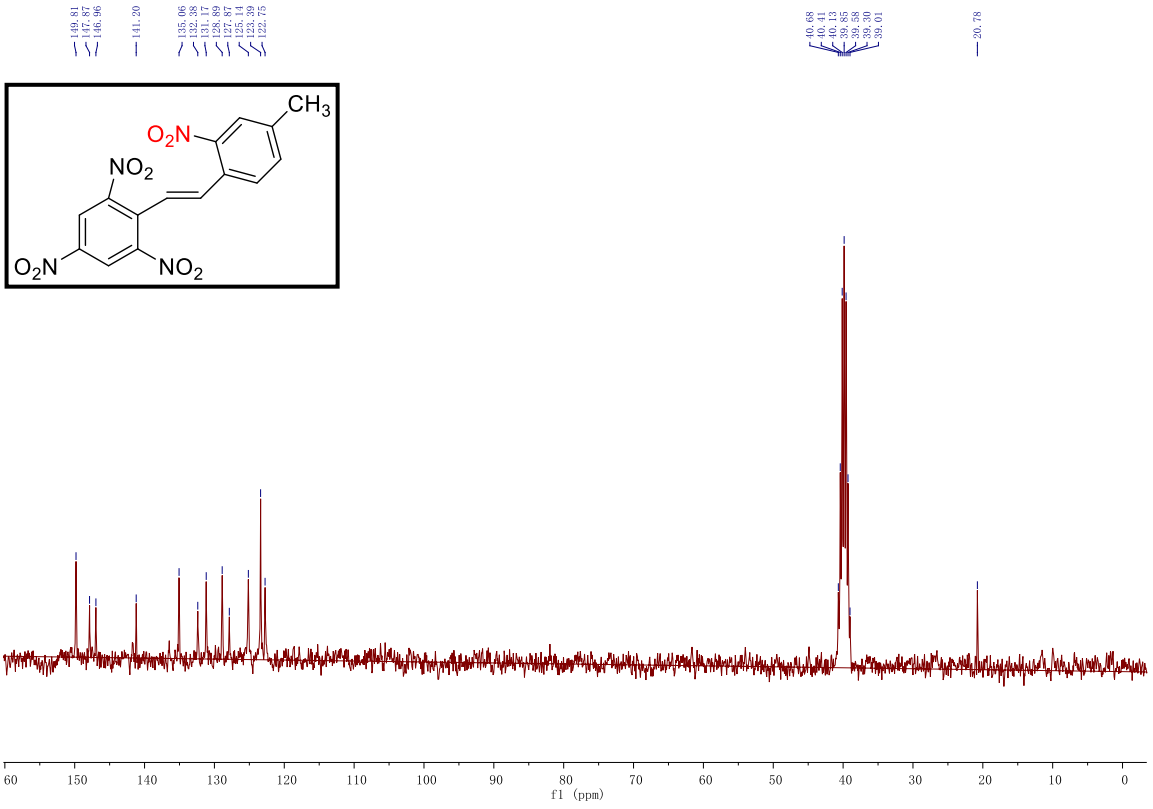

9.14
8.17
8.15
7.57
7.54
7.24
7.23
7.22
7.21
7.20
7.19
3.97
3.35
2.51
2.51
2.51
O2N
NO2
OCH3
O2N
NO2
1.79
1.00
1.03
3.00
3.16
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

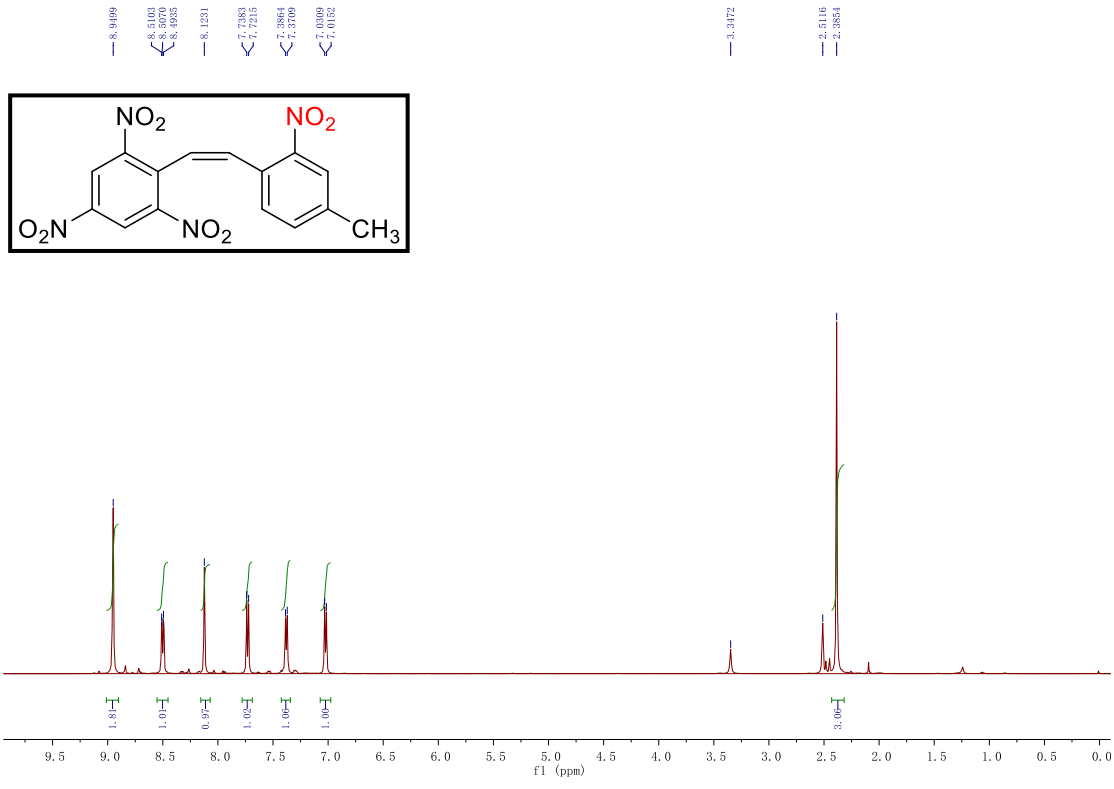

159.02
150.71
145.63
137.95
135.26
130.03
128.99
120.68
119.11
115.07
114.67
111.71
76.31
76.05
75.80
54.39
O2N
NO2
OCH3
O2N
NO2
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

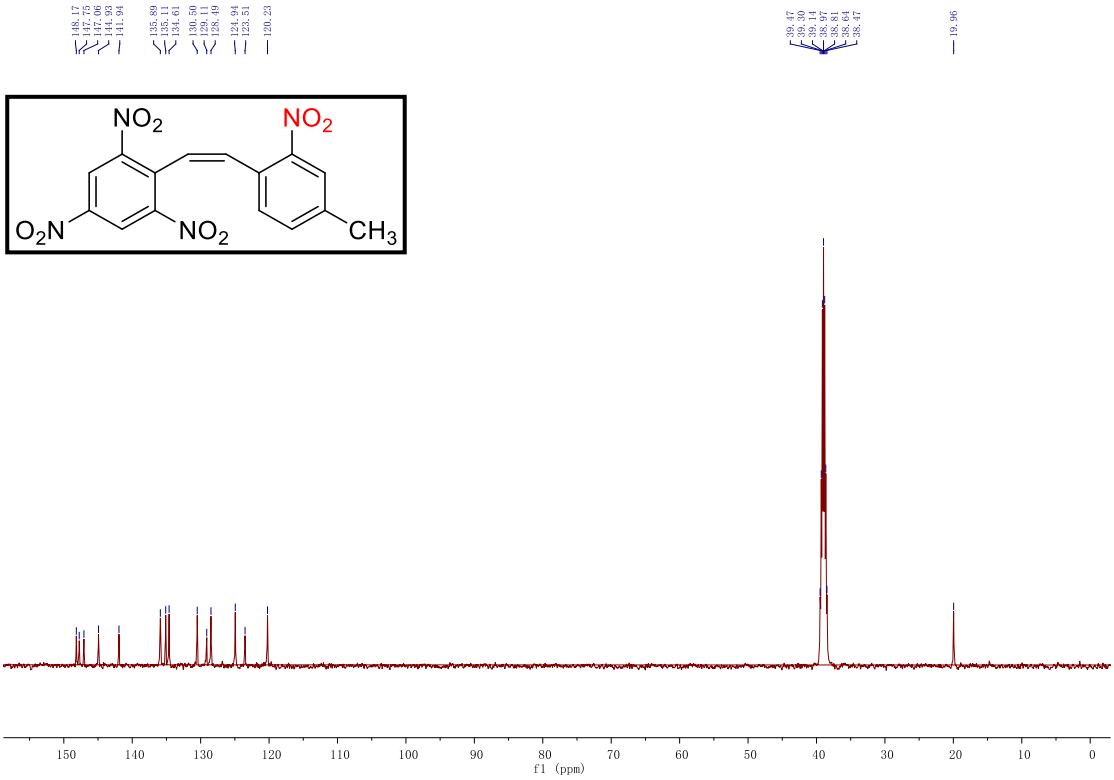

9.15
8.70
7.84
7.79
7.55
7.26
7.20
4.19
3.29
2.49
NO2
O2N
NO2
OCH3
O2N
NO2
1.40
0.73
1.30
1.47
0.96
3.67
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

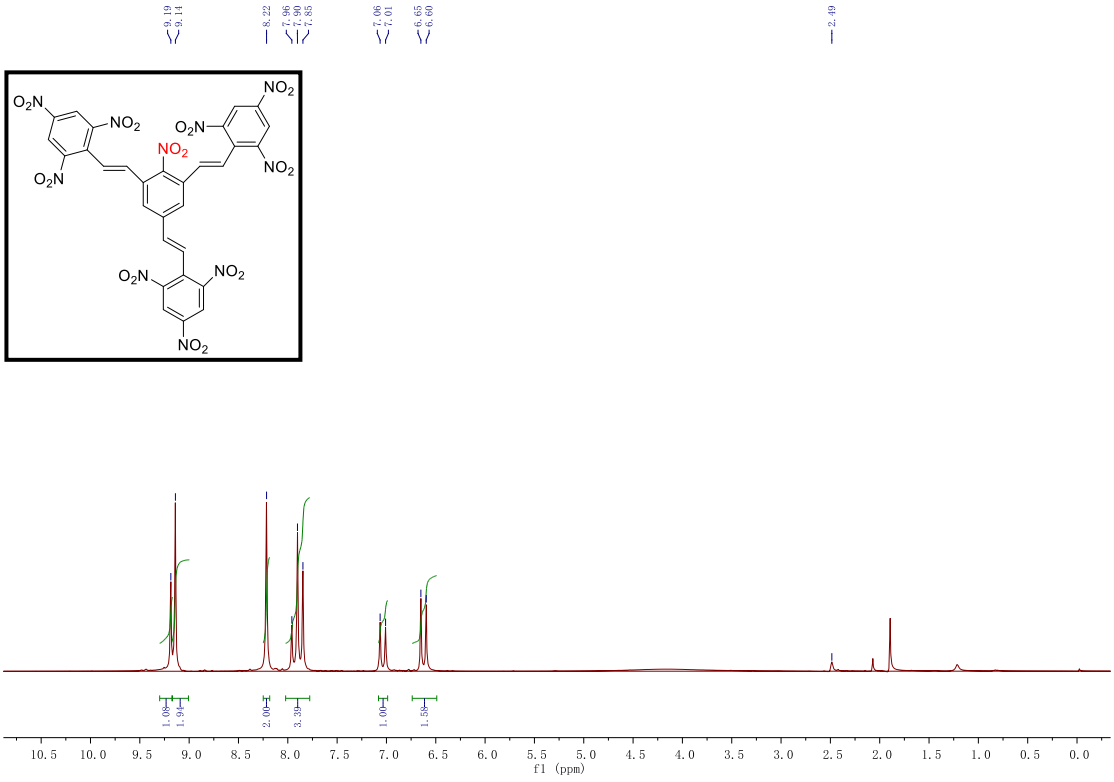

155.75
149.77
147.31
139.34
137.87
131.49
131.97
130.76
126.40
123.67
123.11
114.45
58.18
40.68
40.41
40.13
39.85
39.58
39.30
39.03
NO2
O2N
NO2
OCH3
O2N
NO2
f1 (ppm)

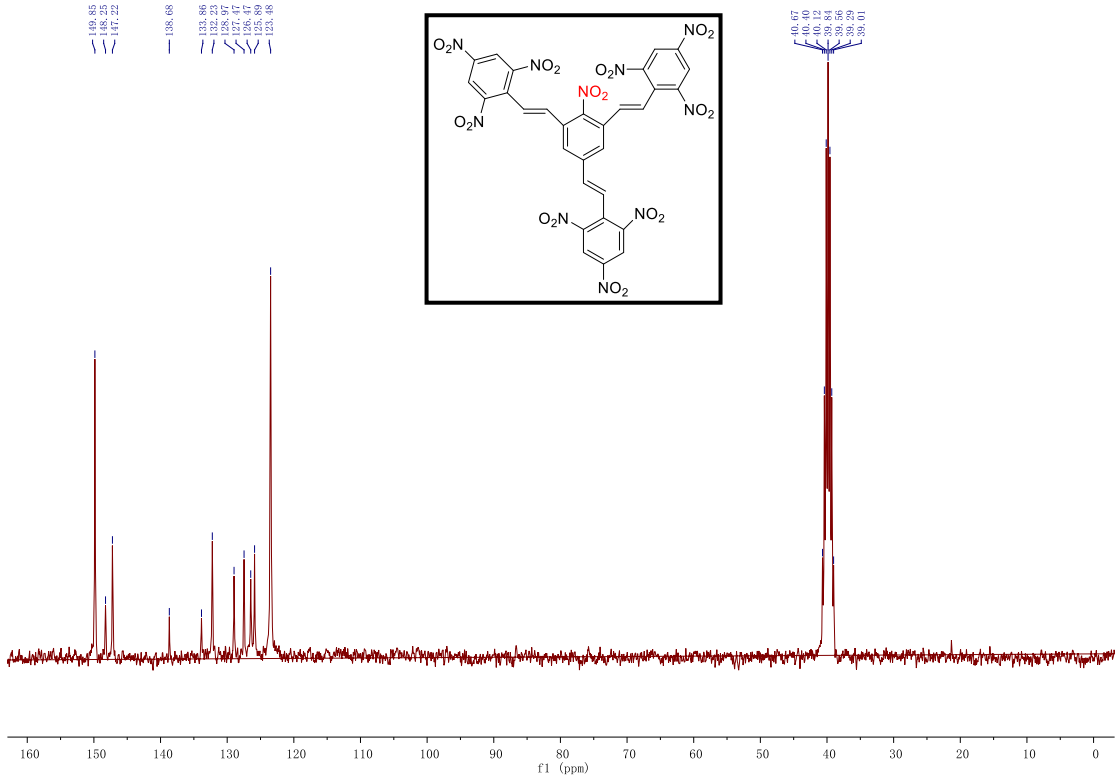

9.11
7.89
7.76
7.74
7.67
7.64
7.51
7.46
7.07
7.02
3.33
2.49
2.42
CH3
O2N
NO2
O2N
NO2
1.27
0.89
1.00
1.01
0.99
0.77
2.97
f1 (ppm)

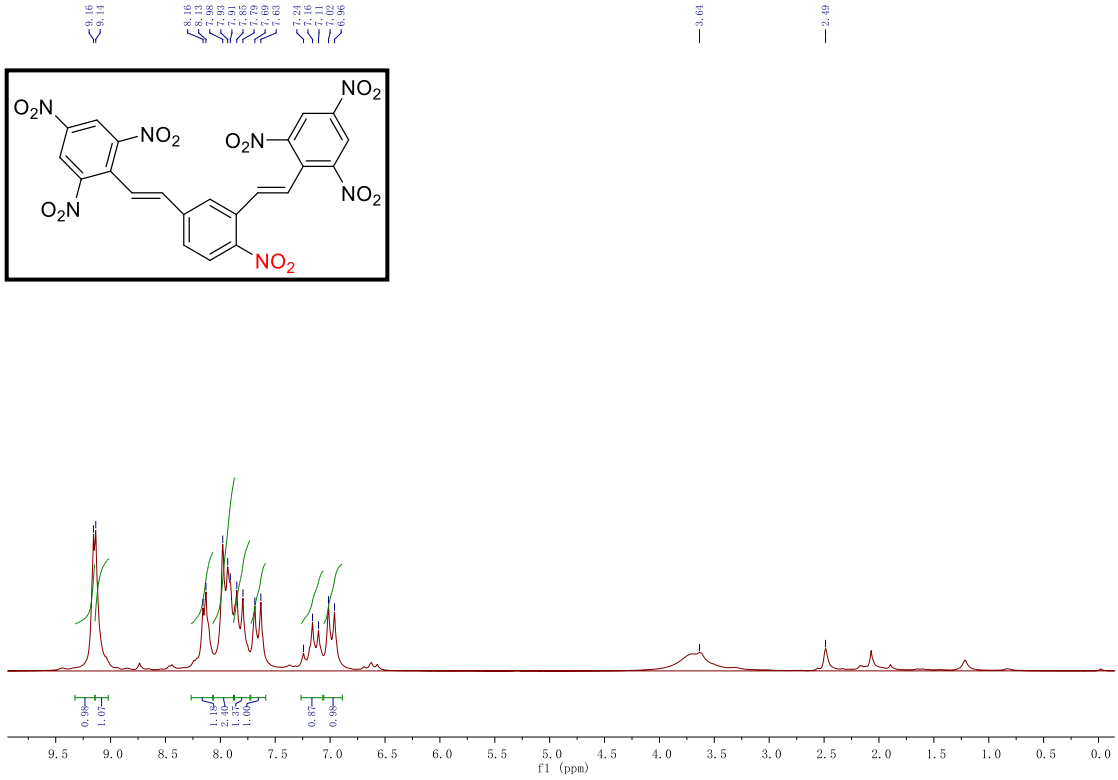

149.81
147.87
146.96
141.20
135.06
132.38
131.17
128.89
127.87
125.14
123.39
122.75
40.68
40.41
40.13
39.85
39.58
39.30
39.01
20.78
CH3
O2N
NO2
O2N
NO2
f1 (ppm)

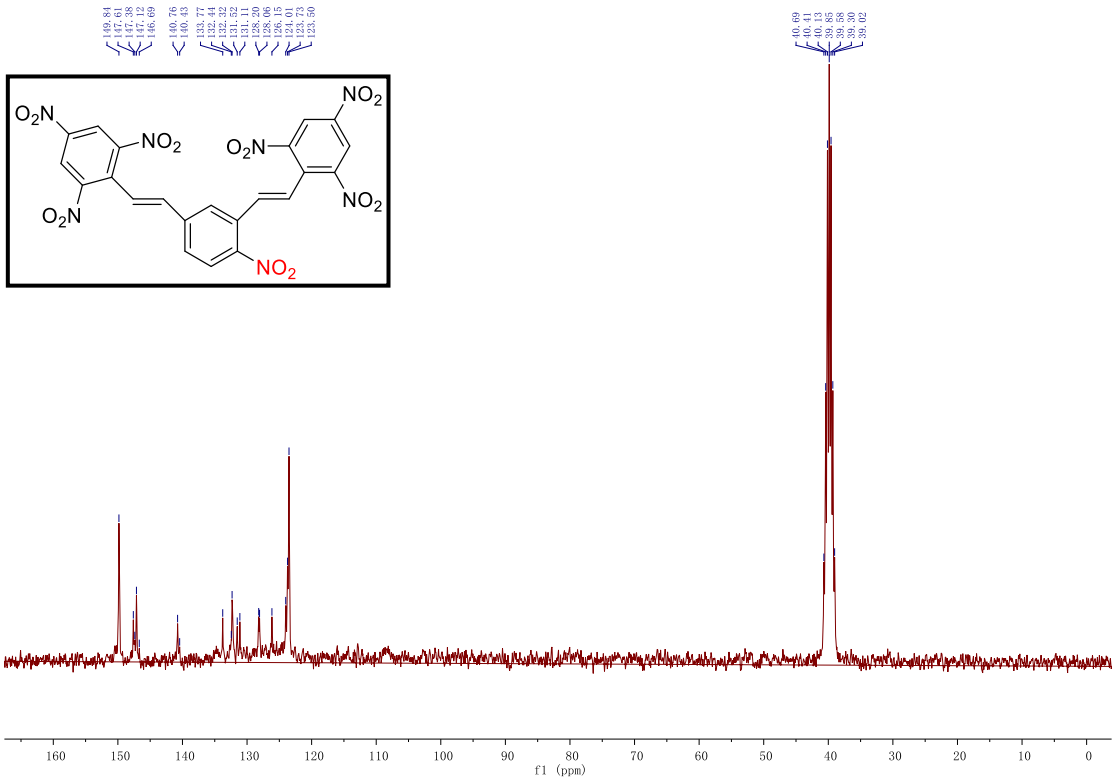

8.9499
8.5103
8.5070
8.4935
8.1231
7.7383
7.7215
7.3864
7.3709
7.0309
7.0152
3.3472
2.5116
2.3854
NO2
NO2
O2N
NO2
CH3
1.81
1.01
0.97
1.02
1.06
1.00
3.06
f1 (ppm)


148.17
147.75
147.06
144.93
141.94
135.89
135.11
134.61
130.50
129.11
128.49
124.94
123.51
120.23
39.47
39.30
39.11
38.97
38.81
38.64
38.47
19.96
NO2
NO2
O2N
NO2
CH3
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.19
9.14
8.22
7.96
7.90
7.85
7.06
7.01
6.65
6.60
2.49
O2N
NO2
NO2
O2N
NO2
O2N
NO2
NO2
O2N
NO2
NO2
1.08
1.94
2.04
3.39
1.00
1.58
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


149.85
148.25
147.22
138.68
133.86
132.23
128.97
127.47
126.47
125.89
124.48
40.67
40.40
40.12
39.84
39.56
39.29
39.01
NO2
O2N
f1 (ppm)


9.16
9.14
8.16
8.13
7.98
7.93
7.91
7.85
7.79
7.69
7.63
7.24
7.16
7.11
7.02
6.96
3.64
2.49
NO2
O2N
0.98
1.07
1.19
2.40
1.37
1.00
0.87
0.98
f1 (ppm)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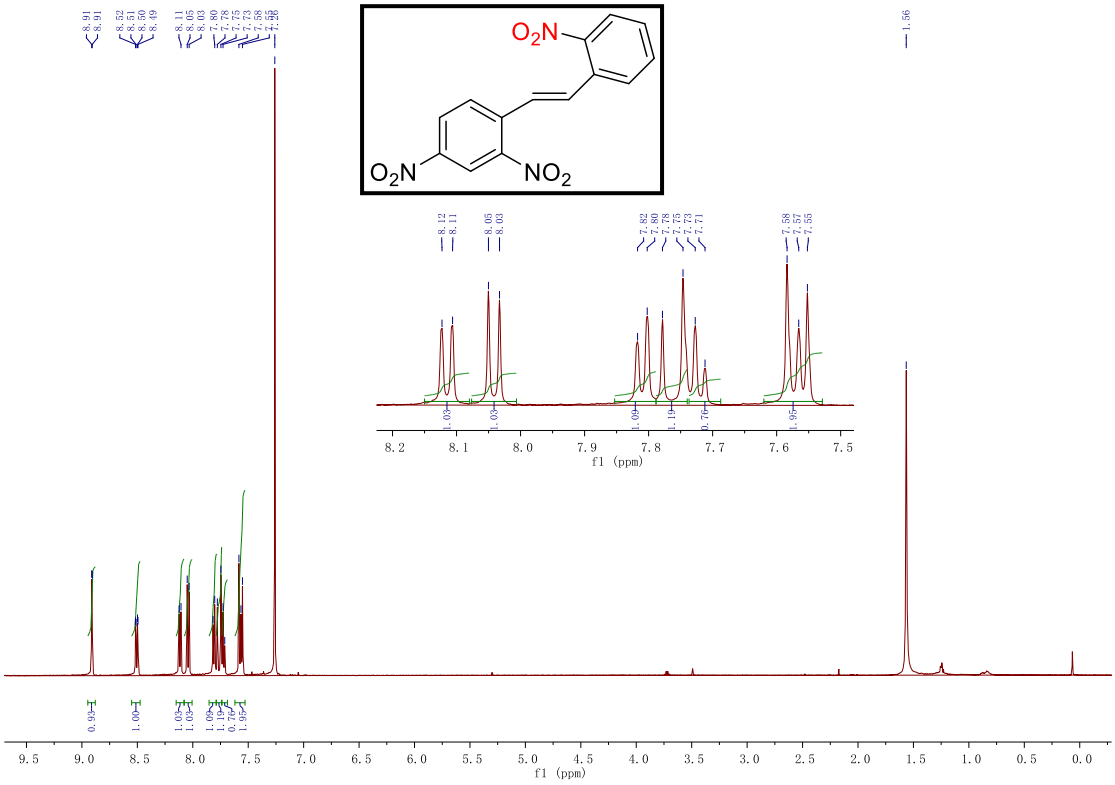
147.12
146.69
140.76
140.43
133.77
132.44
132.32
131.52
131.11
128.20
126.96
126.15
124.01
123.73
123.50
40.69
40.41
40.13
39.85
39.58
39.30
39.02
O2N
NO2
O2N
NO2
O2N
NO2
NO2
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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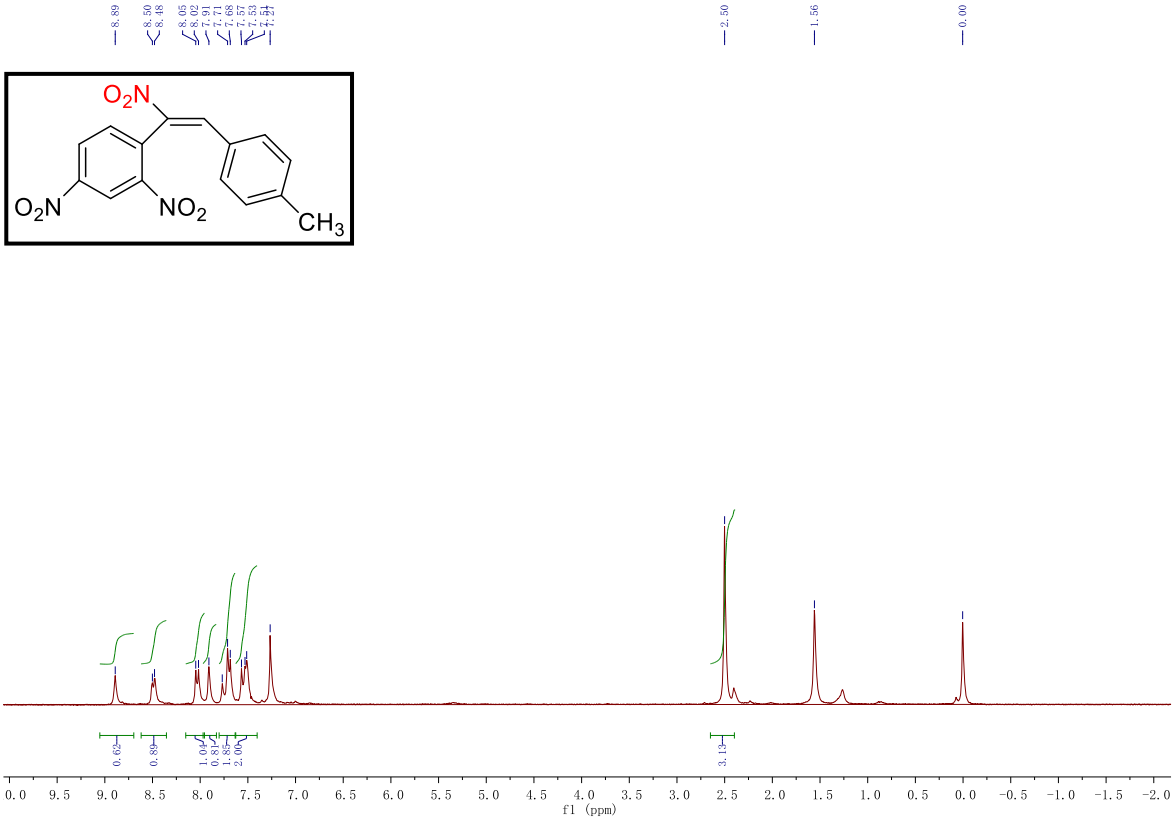
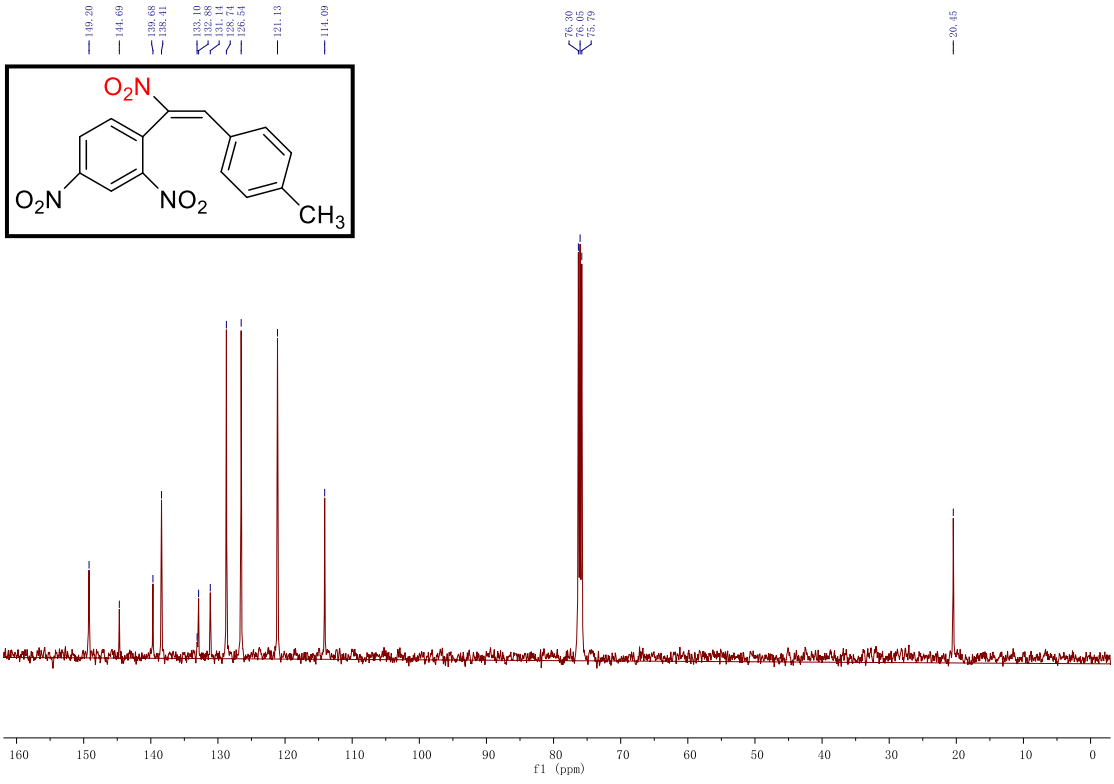
8.91
8.52
8.51
8.50
8.49
8.11
8.05
8.03
7.80
7.78
7.75
7.73
7.68
7.55
7.55
1.56
O2N
O2N
NO2
8.12
8.11
8.05
8.03
7.82
7.80
7.78
7.75
7.73
7.71
7.58
7.57
7.55
1.03
1.00
1.00
1.19
0.70
1.95
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
f1 (ppm)
0.94
1.00
1.03
1.03
1.09
1.19
0.74
1.95
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


8.89
8.50
8.48
8.05
8.02
7.91
7.71
7.68
7.57
7.53
7.24
2.50
1.56
0.00
O2N
O2N
NO2
CH3
0.62
0.89
1.04
0.81
1.85
2.00
3.13
f1 (ppm)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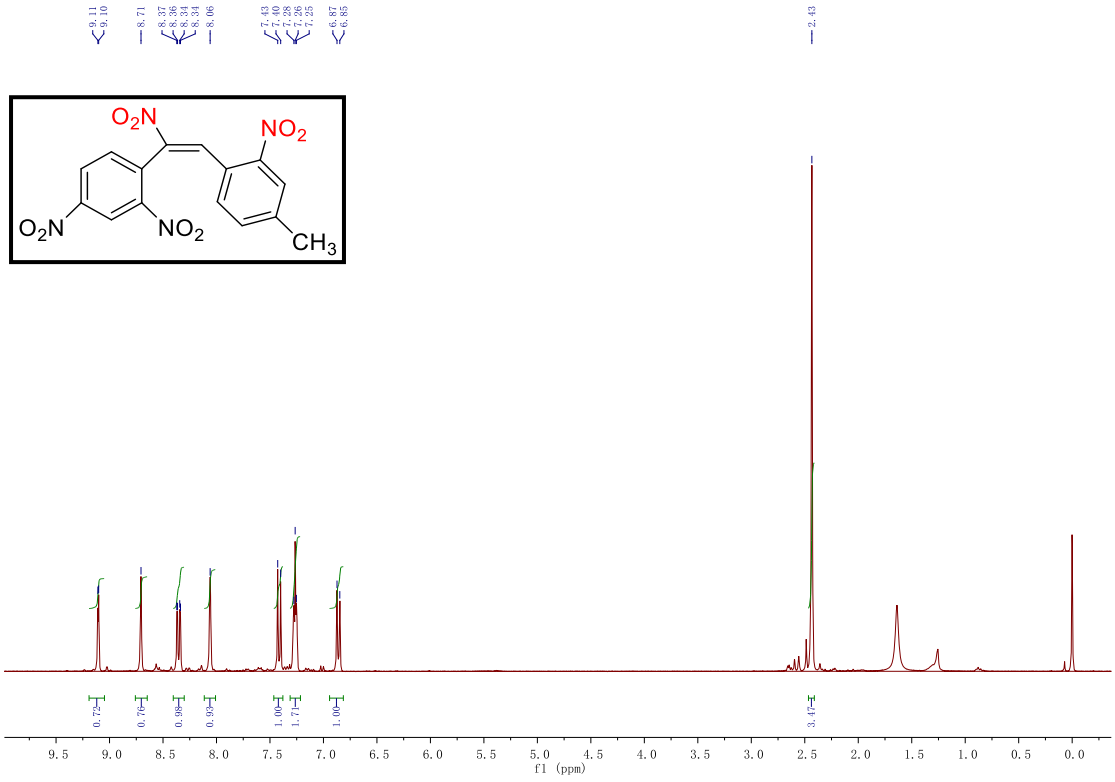
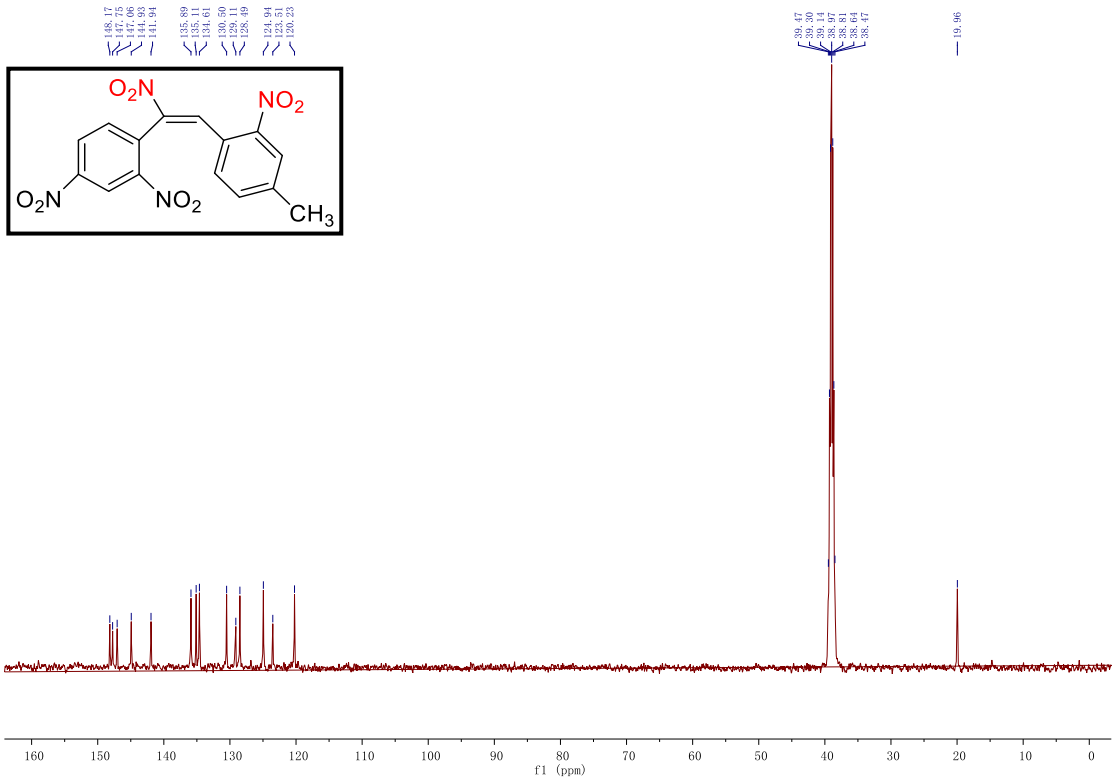
144.69
139.68
138.41
133.10
132.88
131.14
128.74
126.54
121.13
114.09
76.30
76.05
75.79
20.45
O2N
O2N
NO2
CH3
f1 (ppm)


9.11
9.10
8.71
8.37
8.36
8.34
8.33
8.06
7.43
7.40
7.28
7.26
7.25
6.87
6.85
2.43
O2N
NO2
O2N
NO2
CH3
0.72
0.76
0.98
0.93
1.00
1.71
1.00
3.47
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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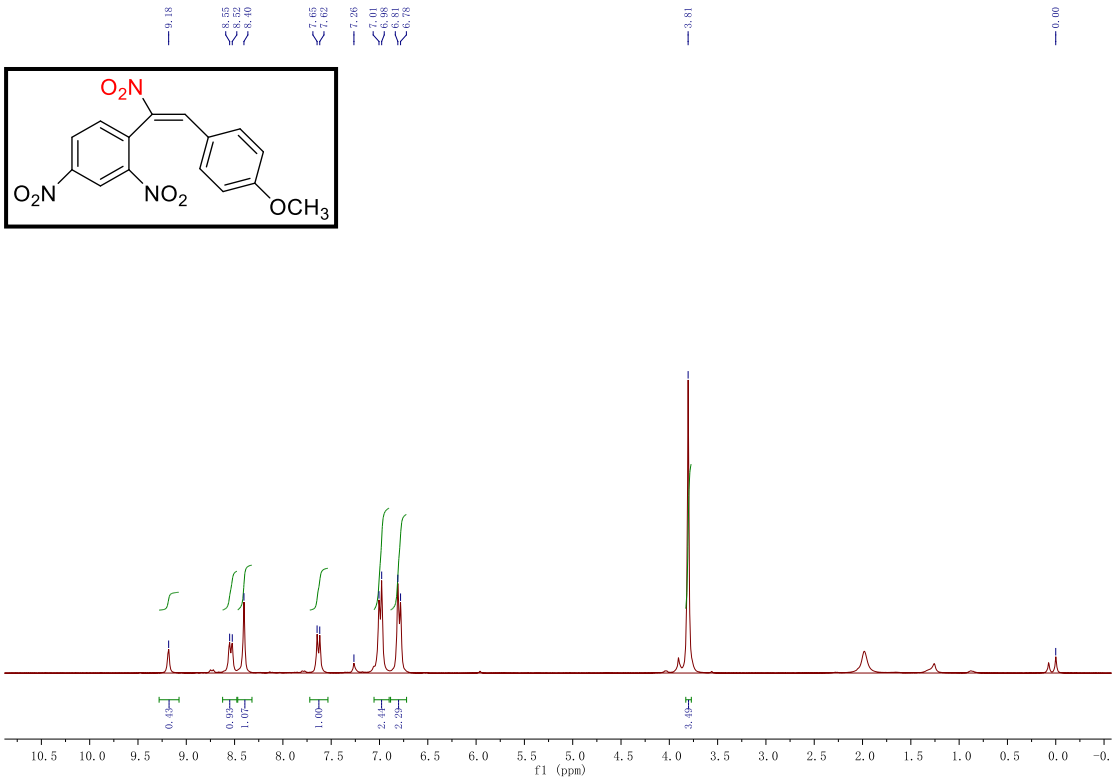
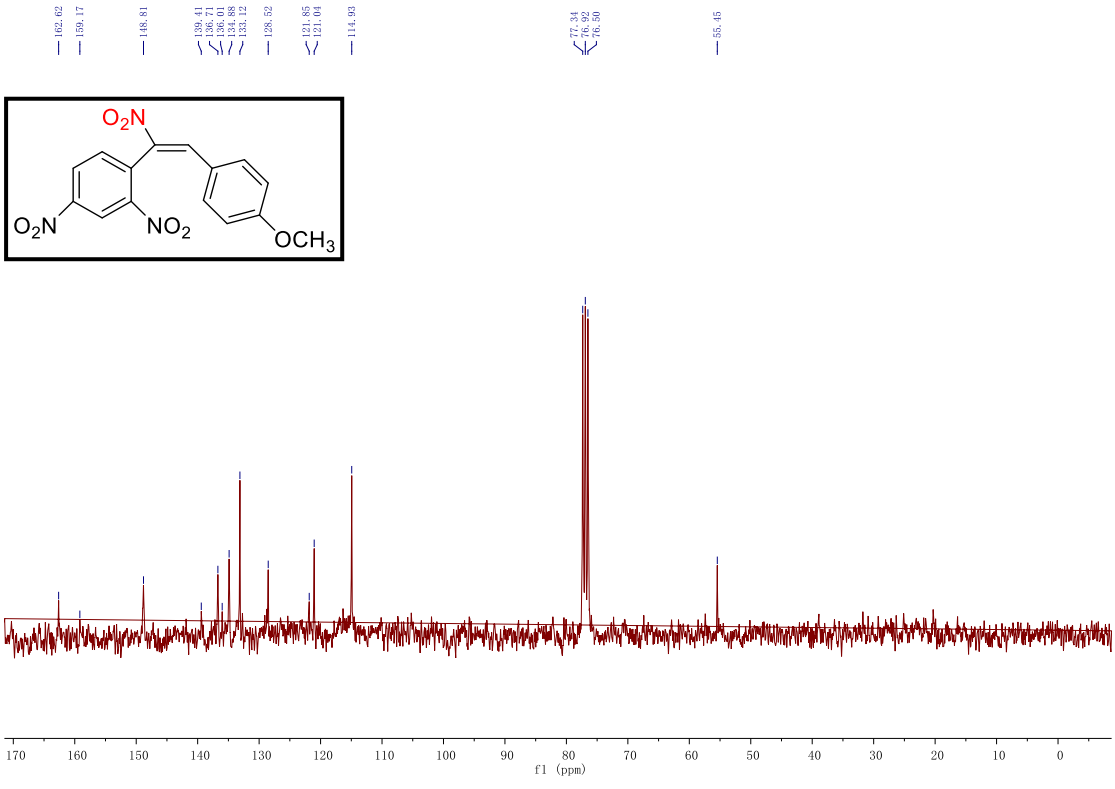
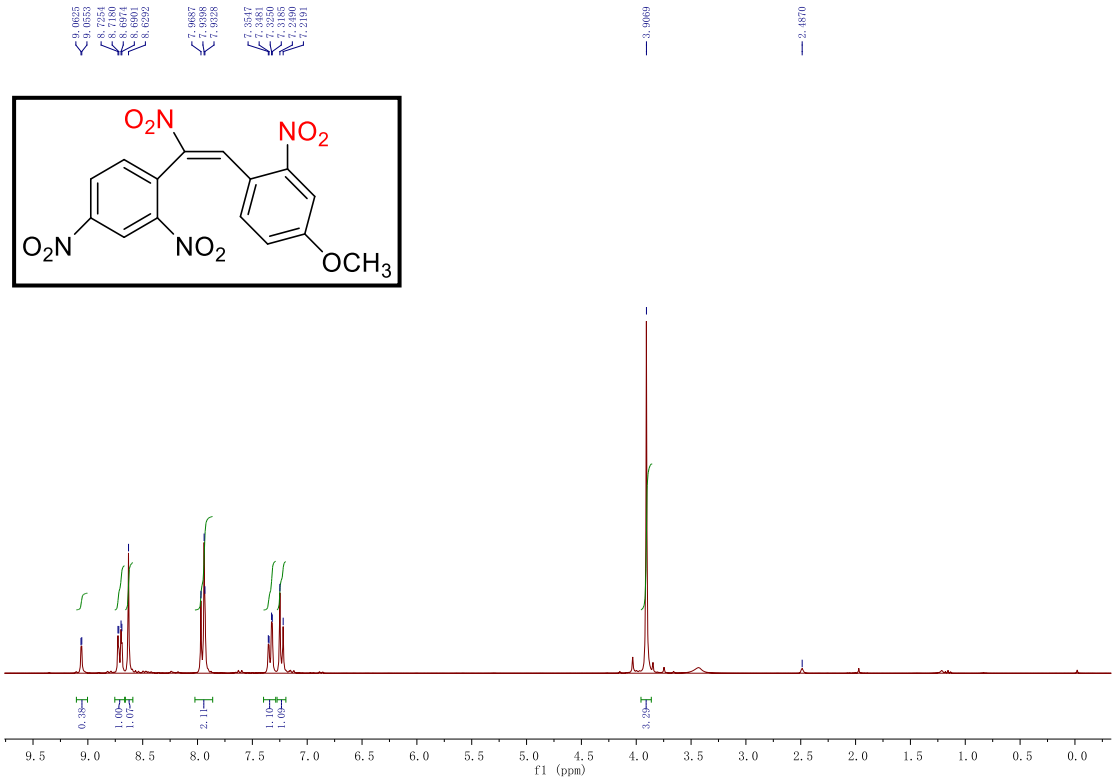
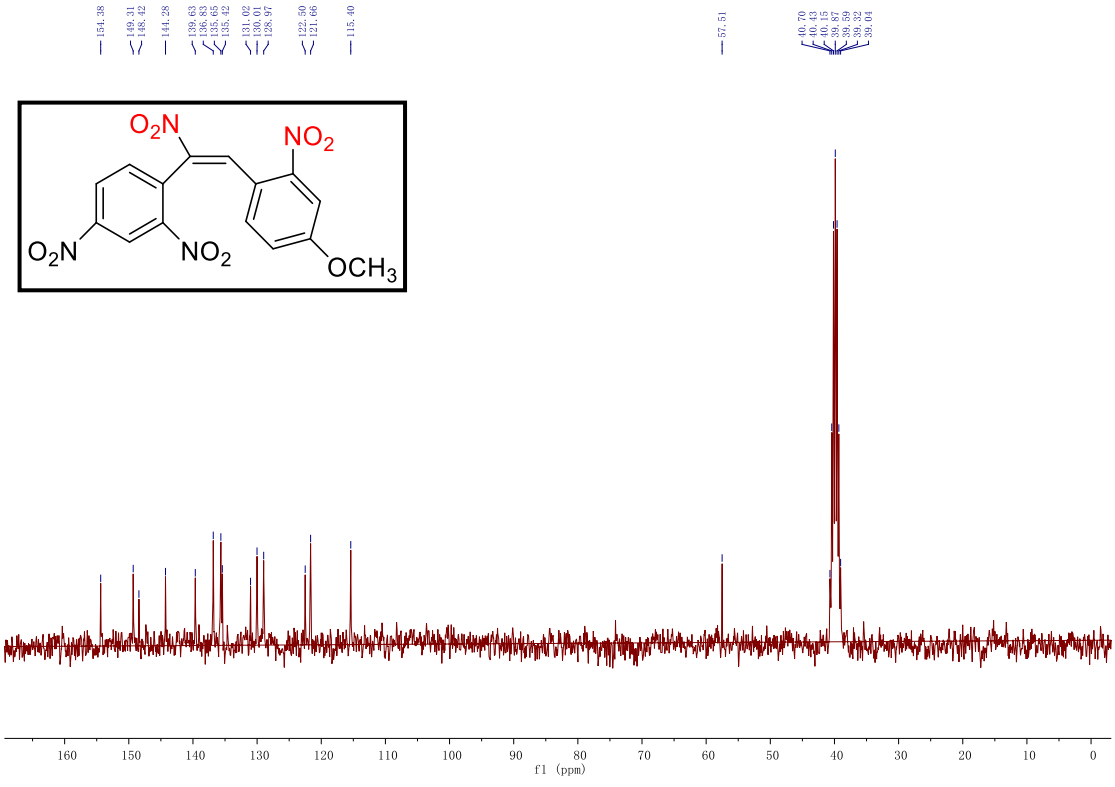
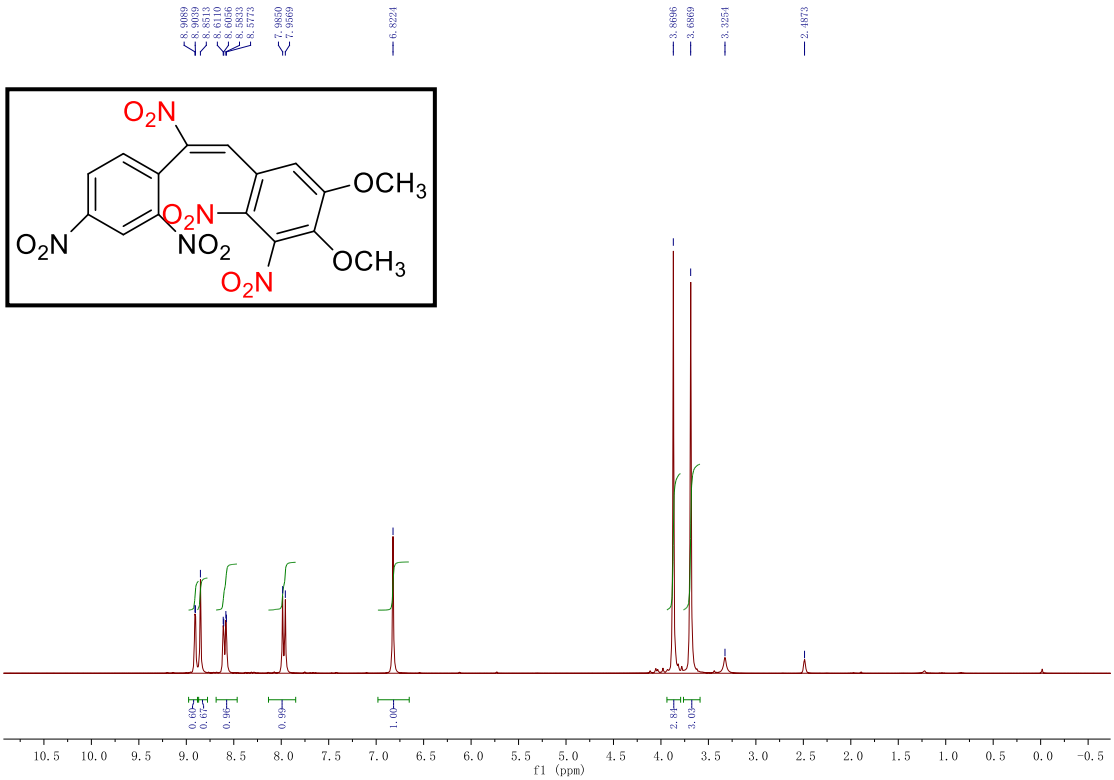
147.75
147.06
144.83
141.94
135.89
135.11
134.61
130.50
129.11
128.49
124.94
123.51
120.23
39.47
39.30
39.14
38.97
38.81
38.64
38.47
19.96
O2N
NO2
O2N
NO2
CH3
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

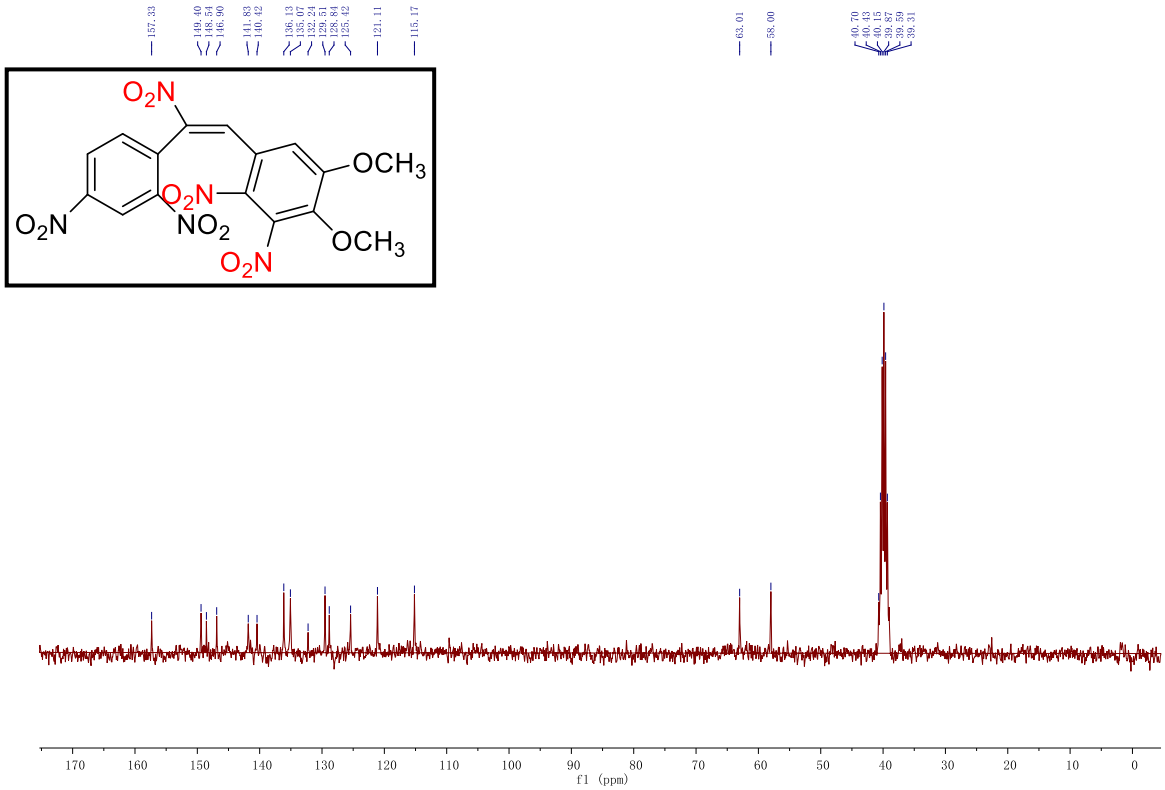

9.18
8.55
8.52
8.40
7.65
7.62
7.26
7.01
6.98
6.81
6.78
3.81
0.00
O2N
O2N
NO2
OCH3
0.43
0.93
1.07
1.00
2.41
2.29
3.40
f1 (ppm)

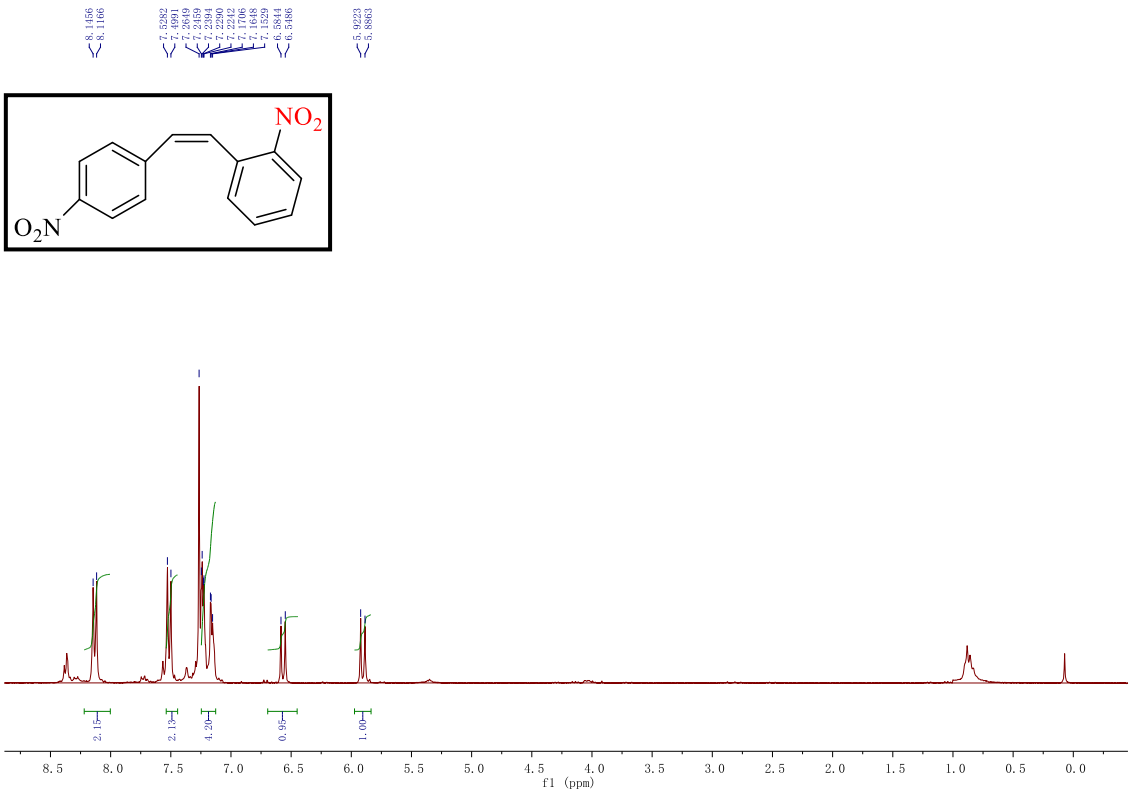

162.62
159.17
148.81
139.41
136.71
136.01
134.88
133.12
128.52
121.85
121.04
114.93
77.34
76.92
76.50
55.45
O2N
O2N
NO2
OCH3
f1 (ppm)

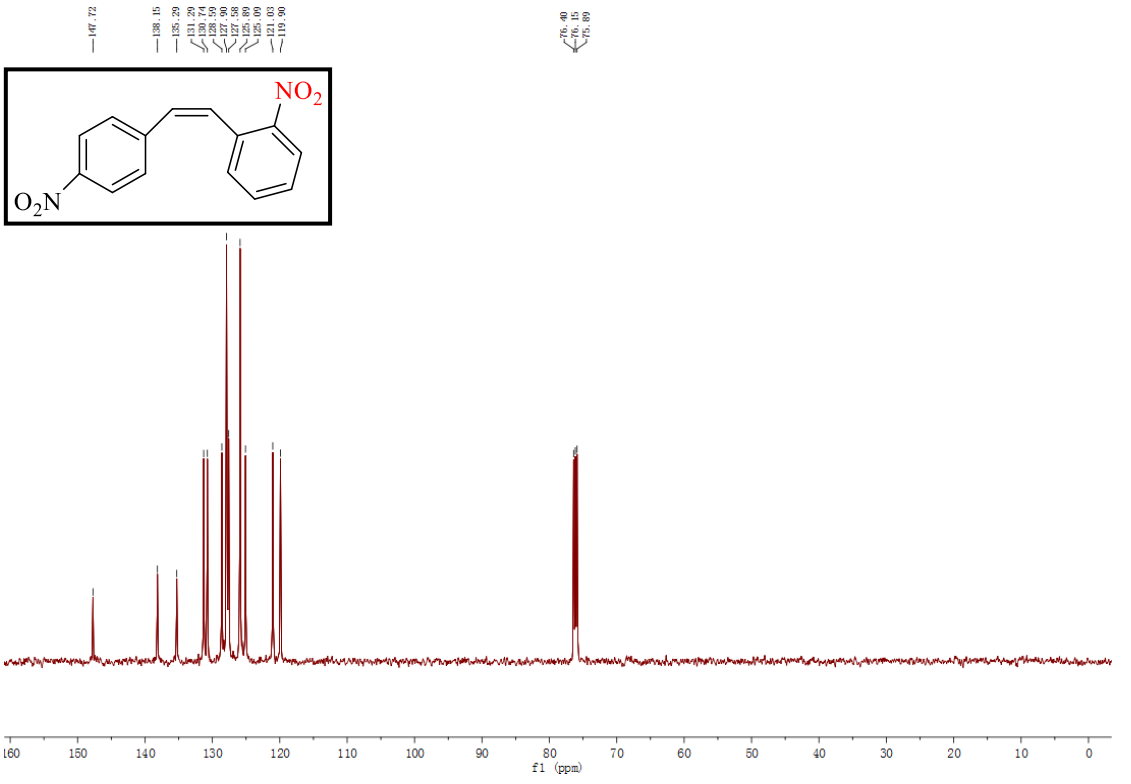

9.0625
9.0553
8.7254
8.7196
8.6974
8.6901
8.6292
7.9687
7.9398
7.9328
7.3547
7.3481
7.3250
7.3185
7.2490
7.2191
3.9069
2.4870
O2N
NO2
O2N
NO2
OCH3
0.38
1.06
1.07
2.11
1.10
1.06
3.29
f1 (ppm)

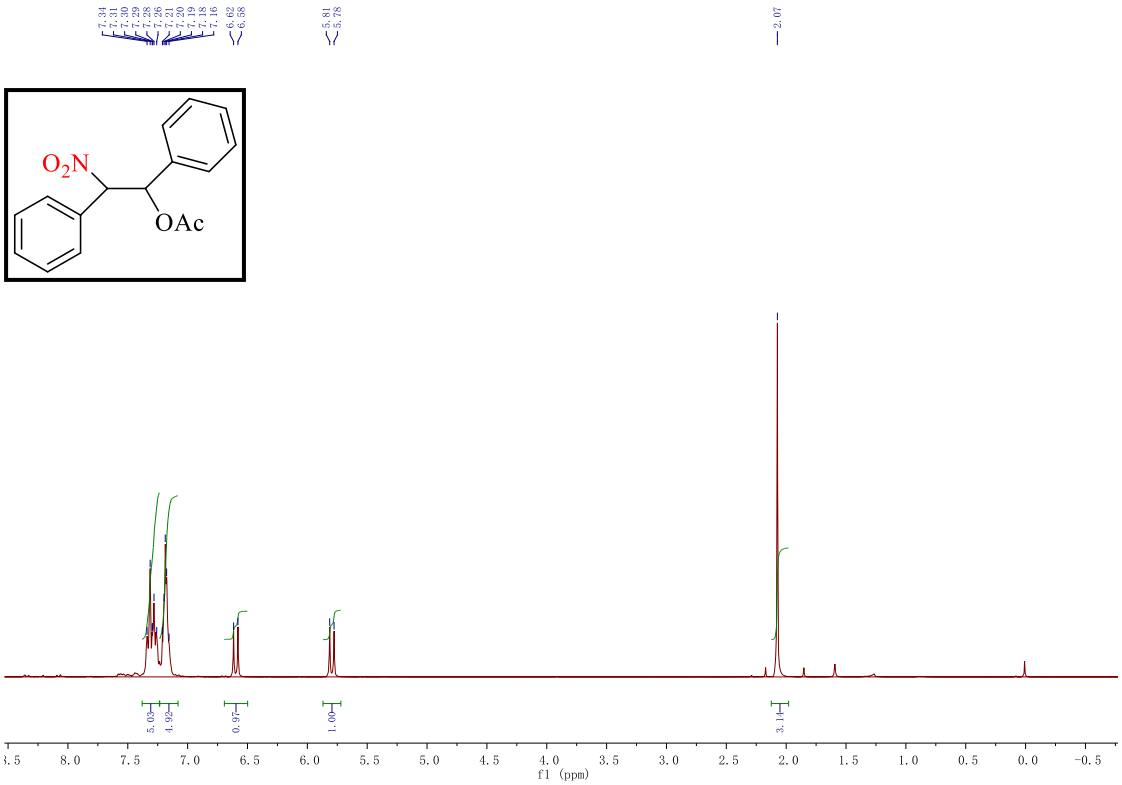

154.38
149.31
148.42
144.28
139.63
136.83
135.65
135.42
131.02
130.01
128.97
122.50
121.66
115.40
57.51
40.70
40.43
40.15
39.87
39.59
39.32
39.04
O2N
NO2
O2N
NO2
OCH3
f1 (ppm)

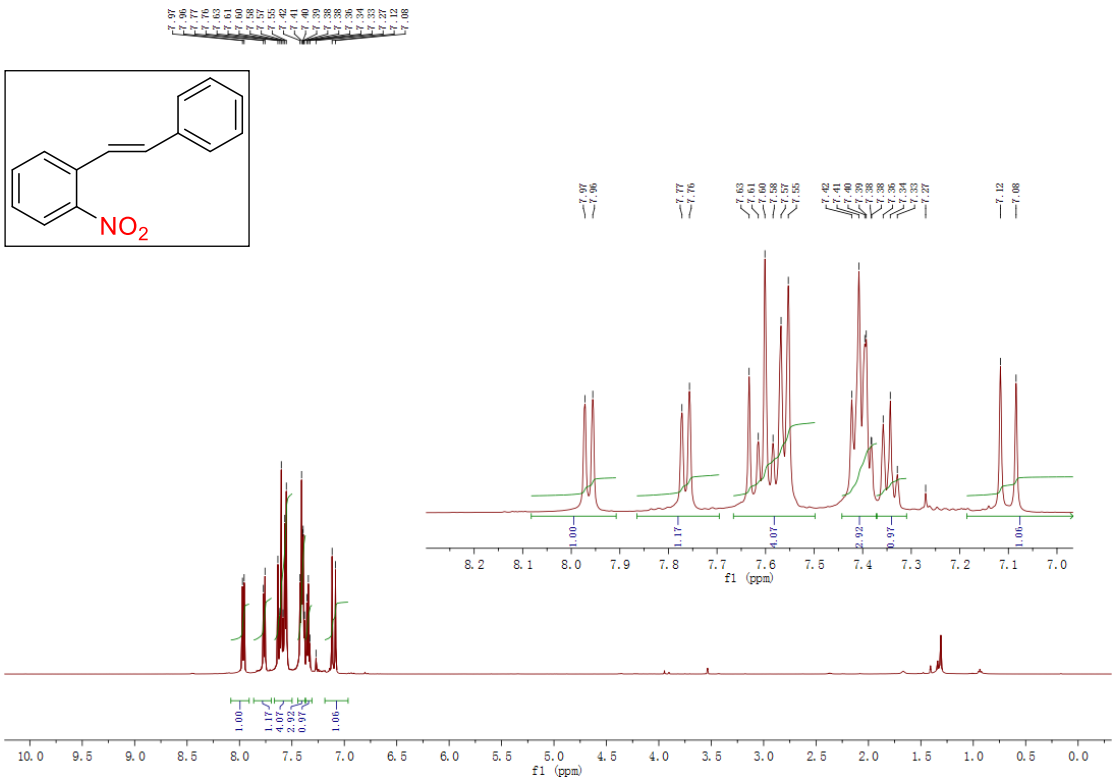

8.9089
8.8813
8.6110
8.6056
8.5783
8.5773
7.9850
7.9569
6.8224
3.8696
3.6869
3.3254
2.4873
O_2N
OCH_3
O_2N
O_2N
NO_2
OCH_3
O_2N
0.60
0.67
0.96
0.99
1.00
2.84
3.03
f1 (ppm)

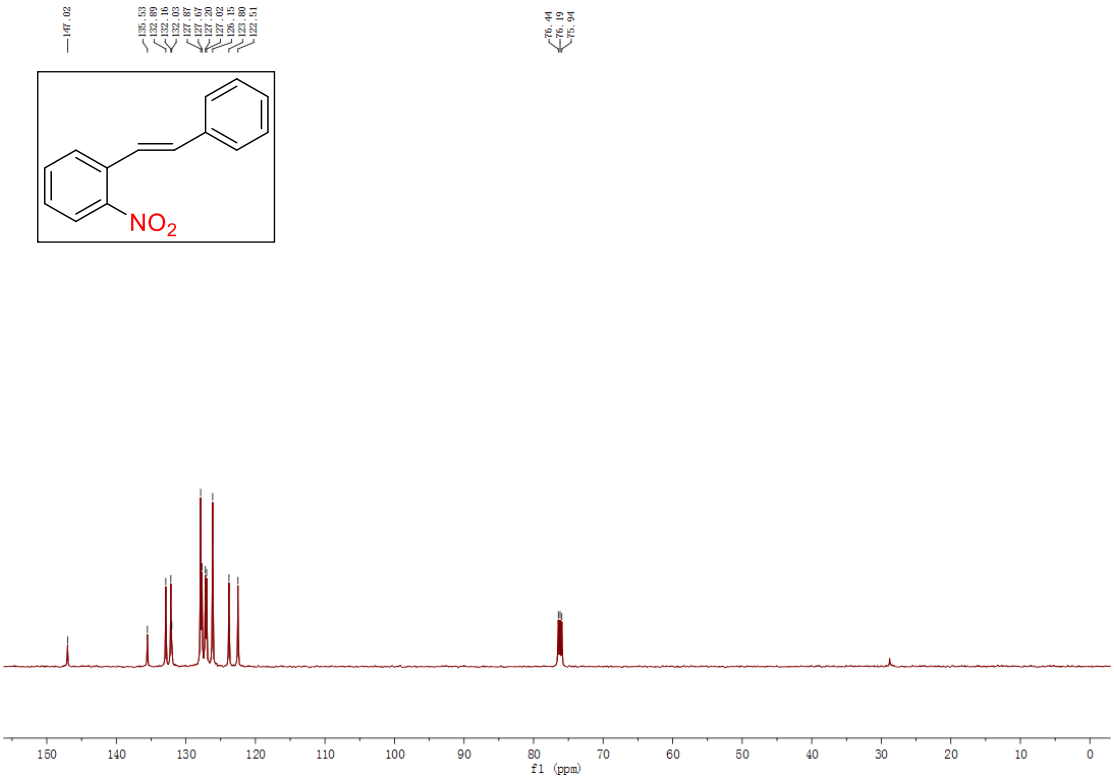

157.33
149.40
148.54
146.90
141.83
140.62
136.13
135.07
132.24
129.51
128.84
125.62
121.11
115.17
63.01
58.00
40.70
40.43
40.15
39.87
39.59
39.31
O_2N
OCH_3
O_2N
O_2N
NO_2
OCH_3
O_2N
f1 (ppm)


8.1456
8.1166
7.5282
7.4991
7.2649
7.2458
7.2394
7.2242
7.2190
7.1706
7.1658
7.1529
6.5844
6.5486
5.9223
5.8863
NO2
O2N
2.15
2.13
4.20
0.95
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


147.72
138.15
135.29
131.29
130.74
128.59
127.90
127.58
125.89
125.09
121.03
119.90
76.40
76.15
75.89
NO2
O2N
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O2N
OAc
f1 (ppm)


NO2
f1 (ppm)


147.02
135.53
132.89
132.16
132.03
127.87
127.57
127.30
127.02
126.15
123.80
122.51
76.44
76.19
75.94
NO2
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

8. References

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